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3-D INELASTIC ANALYSIS METHODS
FOR HOT SECTION COMPONENTS

Third Annual Status Report
For the Period
February 14, 1985 to February 14, 1986

Volume I
Special Finite Element Models

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S. Nakazawa

Contract NAS3-23697
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This Annual Status Report presents the results of work performed during the third year of the 3-D Inelastic Analysis Methods for Hot Section Components program (NASA Contract NAS3-23697). The objective of the program is to produce a series of new computer codes that permit more accurate and efficient three-dimensional analyses of selected hot section components, i.e., combustor liners, turbine blades and turbine vanes. The computer codes embody a progression of mathematical models and are streamlined to take advantage of geometrical features, loading conditions, and forms of material response that distinguish each group of selected components. This report is presented in two volumes. Volume I describes effort performed under Task IVB, "Special Finite Element Special Function Models," while Volume II concentrates on Task IVC, "Advanced Special Functions Models."

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PREFACE

This volume of the Annual Status Report describes the results of work performed on Task IVB (Special Finite Element Models) during the third year of the NASA Hot Section Technology Program, "3-D Inelastic Analysis Methods for Hot Section Components" (Contract NAS3-23697). The goal of the program is to develop computer codes which permit more accurate and efficient structural analyses of gas turbine blades, vanes and combustor liners. The program is being conducted under the direction of Dr. C. C. Chamis of the NASA-Lewis Research Center. Prime contractor activities at United Technologies Corporation are managed by Dr. E. S. Todd. Subcontractor efforts on finite element tasks at MARC Analysis Research are led by Dr. J. C. Nagtegaal.

PROLOGUE

3-D INELASTIC ANALYSIS METHODS FOR HOT SECTION COMPONENTS

VOLUME I - SPECIAL FINITE ELEMENT METHODS

by

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The Special Finite Element Models portion of the 3-D Inelastic Analysis Methods Program is divided into two 24-month segments: a base program, and an option program exercised at the discretion of the Government. Versions 1 and 2 of the MHOST (MARC-HOST) code were developed during the base program (Tasks IB and IIB). The MHOST code employs both shell and solid (brick) elements in an iterative mixed method framework to provide comprehensive capabilities for investigating local (stress/strain) and global (vibration/buckling) behavior of hot section components. In the development of the code, full advantage has been taken of the wealth of technical expertise accumulated at the MARC Corporation over the last decade in support of their own commercially available software package. This has led to the creation of new/improved algorithms that promise to significantly reduce the central processing unit (CPU) time requirements for three-dimensional analyses.

Version 3 of the MHOST code concentrated on algorithm refinement to boost the performance of the basic mixed iterative solution methods; work has also continued on a subelement solution strategy designed to capture local behavior related to embedded discontinuities. Considerable efforts have been devoted to maintaining the computer program and improving the quality of the code, including a substantial number of comment statements in the code. An out-of-core frontal solution subsystem has been made available, in addition to the original band matrix solution, and the MHOST user interface has been modified to make it more user-friendly. An anisotropic material data reader has been added to MHOST as a replacement for the user subroutine option. The shell element definition has also been modified to allow the modeling of composite laminate materials.

TABLE OF CONTENTS

Section Title Page

1.0 INTRODUCTION 1

2.0 SUMMARY 3

3.0 TECHNICAL PROGRESS 4
3.1 Literature Survey 4
  3.1.1 Introduction 4
  3.1.2 Finite Element Approximations 6
    3.1.2.1 Variational Formulations 6
    3.1.2.2 Element Technology 9
  3.1.3 Solution Algorithms 14
  3.1.4 Postprocessing 16
  3.1.5 Conclusions 18
3.2 Global Solution Strategy and Element Technology 20
  3.2.1 Introduction 20
  3.2.2 The Augmented Hu-Washizu Formulation 20
  3.2.3 Iterative Algorithms 21
  3.2.4 Nonlinear Solution Processes 26
  3.2.5 Element Technology 31
    3.2.5.1 Element Integration Procedures 31
    3.2.5.2 Coordinate Transformations 31
3.3 Local Analysis Procedures 32
  3.3.1 Introduction 32
  3.3.2 Crack Tip Singularity and Special Function Expansion 33
  3.3.3 Coding Strategy 38
3.4 Computer Code Development and Validation 39
  3.4.1 Introduction 39
  3.4.2 Solution Capabilities 39
  3.4.3 Solution Algorithms 48
  3.4.4 Frontal Solution Subsystem 53
  3.4.5 Anisotropic Material Property Reader 57
    3.4.5.1 Composite Laminate Option 57
    3.4.5.2 Anisotropic Elastic Material Reader 62
  3.4.6 Coordinate Transformations 62
  3.4.7 Subelement Development 63
3.5 List of Symbols 79
3.6 References 82

LIST OF ILLUSTRATIONS

Figure Number	Title	Page
1	A Beam Problem - Linear Plastic Analysis	49
2	A Three-Dimensional Shell Problem	50
3	A Beam Problem - Elastic Plastic Analysis	51
4	MARC Blister Specimen Model	56
5	Mises Stress for Blister Specimen	57
6	Composite Beam Model Geometry and Finite Element Mesh	61
7	MHOST Selective Integration Versus Pian Rational Hybrid Stress	63
8	Problem Statement for Plane Stress Deformation of a Domain with a Singularity	65
9	Three-Dimensional Subelement Validation	68
10	Subelement Refinement for the Beam Problem	69
11	Finite Element Mesh for a Hole in a Plate	70
12	Stress Distribution Along the Edge A - B Global Mixed Solution with Coarse Mesh	71
13	Mises Equivalent Stress Global Mixed Solution with Coarse Mesh	71
14	Stress Distribution Along the Edge A - B: Coarse Mesh with Linear-Quadratic Subelement Division	72
15	Mises Equivalent Stress: Coarse Mesh with Linear-Quadratic Subelement Division	72
16	Subelement Mesh for a Hole	74
17	Global Finite Element Mesh	74
18	Standard Finite Element Model with a Hole	75

LIST OF TABLES

Table Number	Title	Page
I	MHOST Code, Version 3.2 Elements and Parameters	43
II	Elastic Beam: Convergence with Respect to Iteration	49
III	A Three-Dimensional Shell Problem: Convergence with Respect to Iteration	50
IV	Solution of the Elastic Plastic Beam Problem	52
V	Elastic Beam: Convergence of Modified Line Search, Conjugate Gradient and Secant Newton Procedures	53
VI	Performance Tests for Frontal Solution Subsystem	55
VII	Convergence of the Global Iteration for the Elastic Analysis of the L-Shape Domain (Prescribed Relative Residual Tolerance 0.01)	66
VIII	Stress and Displacement Solution: L-Shape Domain	67
IX	Stresses at the Re-Entrant Corner	68
X	Beam Problem: Subelement Validation	69
XI	Elastic Stress Analysis of a Plate and a Hole: Stress and Strain at the Edge (Point A on Figure 10)	73
XII	Nodal Stress at the Edge of the Circular Hole	76
XIII	Isotropic and Anisotropic Plastic Response of a Cantilever Beam	78

SECTION 1.0

INTRODUCTION

Aircraft powerplant fuel consumption and expenditures for repair/replacement of worn or damaged parts make up a significant portion of commercial aviation's direct operating costs. For modern gas turbines, both factors depend heavily on the degree to which elevated flowpath temperatures are sustained in the hot section modules of the engine. Higher temperatures reduce fuel consumption by raising the basic efficiency of the gas generator thermodynamic cycle. At the same time, these elevated temperatures work to degrade the durability of structural components (combustor liners, turbine blades and vanes, airseals, etc.) that must function adjacent to or within the hot gaspath itself, leading in turn to larger maintenance/material costs. Pursuit of the best compromise between performance and durability presents a challenge that will continue to tax the ingenuity of advanced gas turbine design analysts for years to come.

Hot section durability problems appear in a variety of forms, ranging from oxidation/corrosion, erosion, and distortion (creep deformations) to occurrence of fatigue cracking. Even modest changes in shape, from erosion or distortion of airfoils for example, can lead to measurable performance deterioration that must be accurately predicted during propulsion system design to ensure that long-term efficiency guarantees can be met. Larger distortions introduce serious problems such as hot spots and profile shifts resulting from diversion of cooling air, high vibratory stresses associated with loose turbine blade shrouds, difficult disassembly/reassembly of mating parts at overhaul, etc. These problems must be considered and efforts made to eliminate their effects during the engine design/development process. Initiation and propagation of fatigue cracks represents a direct threat to component structural integrity and must be thoroughly understood and accurately predicted to ensure continued safe and efficient engine operation.

Accurate prediction of component fatigue lives is strongly dependent on the success with which inelastic stress/strain states in the vicinity of holes, fillets, welds, and other discontinuities can be calculated. Stress/strain computations for hot section components are made particularly difficult by two factors: the high degree of geometrical irregularity which accompanies sophisticated cooling schemes, and complex nonlinear material behavior associated with high temperature creep/plasticity effects. Since cooling air extraction reduces engine cycle efficiency, concerted efforts are made to minimize its use with the result that elaborate internal passages and surface ports are employed to selectively bathe local regions (airfoil leading edges, louver liner lips, etc.) for which the high temperature environment is most severe. These cooling features frequently interrupt load paths and introduce complex temperature gradients to the extent that the basic assumptions of one- and two-dimensional stress analysis procedures are seriously compromised and the use of three-dimensional techniques becomes mandatory. Even in the presence of cooling, component temperature and stress levels remain high relative to the material's melting point and yield strength values. The combinations of centrifugal, aerodynamic, thermal, and other mechanical loadings that typically occur in flight operation then serve to drive the underlying material response beyond accepted limits for linear elastic behavior and into the regime characterized by inelastic, time-dependent structural deformations. Thus, an ability to account for both complexities, three-dimensional and inelastic effects, becomes essential to the design of durable hot section components.

General purpose finite element computer codes containing a variety of three-dimensional (brick) elements and inelastic material models have been available for more than a decade. Incorporation of such codes into the hot section design process has been severely limited by high costs associated with the extensive labor/computer/time resources required to obtain reasonably detailed results. Geometric modeling systems and automated input/output data processing packages have received first attention from software developers in recent years and will soon mature to the point that previous over-riding manpower concerns will be alleviated. Prohibitive amounts of central processing unit (CPU) time are still required for execution of even modest-size three-dimension inelastic stress analyses, however, and is chief among the obstacles remaining to be remedied. With today's computers and solution algorithms, models described by a few hundred displacement degrees-of-freedom commonly consume one to three hours of mainframe CPU time during simulation of a single thermomechanical loading cycle. A sequence of many such cycles may, of course, be needed to reach the stabilized conditions of interest. Since accurate idealizations of components with only a few geometrical discontinuities can easily contain several thousand degrees-of-freedom, inelastic analysis of hot section hardware with existing codes falls outside the realm of practicality.

The Inelastic Methods Program addresses the need to develop more efficient and accurate three-dimensional inelastic structural analysis procedures for gas turbine hot section components. A series of new, increasingly rigorous, stand-alone computer codes is being created for the comprehensive numerical analysis of combustor liners, turbine blades and vanes. One of these stand-alone computer programs is based on special finite element models. Heavy attention is being given to the evolutionary development of novel finite element modeling methods that permit non-burdensome yet accurate representations of geometrical discontinuities such as cooling holes and coating cracks. A selection of constitutive relations is being provided for either economical or sophisticated descriptions of inelastic material behavior as desired. The advantages which accrue from application of the improved finite element code being developed under this contract are demonstrated by execution of benchmark analyses for which experimental data exist as well as by efficiency comparisons with other commonly available finite element programs.

SECTION 2.0

SUMMARY

The Special Finite Element Models portion of the 3-D Inelastic Analysis Methods program is divided into two 24-month segments: a base program, and an option program to be exercised at the discretion of the Government. Versions 1 and 2 of the MHOST (MARC-HOST) code were developed during the base program (Tasks IB and IIB). The MHOST code employs both shell and solid (brick) elements in an iterative mixed method framework to provide comprehensive capabilities for investigating local (stress/strain) and global (vibration, buckling) behavior of hot section components. In the development of the code, full advantage has been taken of the wealth of technical expertise accumulated at the MARC Corporation over the last decade in support of their own commercially available software package. This has led to the creation of new/improved algorithms that promise to significantly reduce the central processing unit (CPU) time requirements for three-dimensional analyses.

Version 3 of the MHOST code has been developed under Task IVB of the 3-D Inelastic Analysis Methods option program. The development efforts have concentrated on algorithm refinement to boost the performance of the basic mixed iterative solution method; work has also continued on a subelement solution strategy designed to capture local behavior related to embedded discontinuities.

Considerable efforts have been devoted to maintaining the computer program and improving the quality of the code, including a substantial number of comment statements in the code. An out-of-core frontal solution subsystem has been made available, in addition to the original band matrix solution, and the MHOST user interface has been modified to make it more user-friendly.

At the request of the NASA Program Manager, an anisotropic material data reader has been added to MHOST as a replacement for the user subroutine option. The shell element definition has also been modified to allow the modeling of composite laminate materials.

Algorithmic development for the mixed global solution strategy and local solution techniques as well as computer program development are discussed in detail in Section 3 of this report.

SECTION 3.0

TECHNICAL PROGRESS

3.1 Literature Survey

This section reviews currently available literature on numerical technology with special emphasis on the application of finite elements to nonlinear problems. The main objective is to survey the present state of the art.

Papers, reports and books published after 1980 are included in this survey in conjunction with a few historically significant references published earlier.

3.1.1 Introduction

The finite element method has become a standard tool for numerically simulating a wide range of engineering problems using well-established technology and commercially available software. The numerical methods have been developed continuously in parallel with progress in mathematical theory and hardware technology. The solution of three-dimensional nonlinear problems still remains costly. Analyses with sufficient resolution could be prohibitively expensive without major improvements in numerical and computational methodology.

A major thrust in research and development in the present decade is to refine the algorithms and approximations in order to improve the computational performance of the finite element method. A significant development in the last decade is the penetration of this numerical technology into new engineering fields of applications as summarized in the treatise by Zienkiewicz (1977). This book is currently being revised to include some of the major results of the present decade.

Problems tackled by the finite element method which require new developments are generally nonlinear, multi-dimensional and often subjected to complicated constraint equations and inequalities. Standard technology is often inappropriate or impractical due to the limitations of hardware performance: speed and storage capacity. Research efforts concentrated on the following areas to fully exploit the computational resources:

1. Variational formulations and discretization processes

   Organized "variational crimes" were committed in the past just to make the displacement method operational. These crimes are now legalized by virtue of various mixed and hybrid formulations. The use of the Hu-Washizu principle now provides a firm variational foundation for modern finite element technology. The patch test has also been investigated in the mixed and hybrid methods contexts in recent literature. Augmented forms of the variational statement, which are used to construct numerical solution processes for constrained problems, appear in modern finite element literature.

2. Global solution procedures for linear and nonlinear finite element equations

   As an alternative to factorization of the global stiffness equations, the utilization of iterative solution algorithms has gained popularity. The research effort is concentrated on constructing inexpensive, yet accurate preconditioners in such processes. The iterative solution methods developed for linear and nonlinear programming are used to solve nonlinear finite element equations, as found in papers and reports published recently.

3. Postprocessing techniques including stress smoothing, a posteriori error estimates and adaptive mesh refinement

   Technology to extract extra information from a finite element displacement solution has been developed with a focus on algorithms designed to recover the stress accurately. In addition, research in the underlying variational theory has made notable progress. Error estimates and indicators based on the solution are now available with rigorous mathematical theory. These postprocessing techniques lead to the development of mechanisms to adaptively refine finite element meshes.

Branches of engineering in which the finite element method is applied have diversified to include fluid mechanics and transport phenomena of heat and mass, among many others. The emphasis in this report is on solid and structural mechanics including basic mathematical and numerical ideas and technology specific to this field. Application to three-dimensional inelastic solutions for turbine engine hot section components subjected to realistic thermal and mechanical loading cycles is of special interest. The main cause of difficulties here involves the complicated material response under high temperature and pressure. As summarized by Thompson (1982), the constitutive laws built for monolithic alloys are not simple under practical operating conditions. Introduction of composites such as fiber reinforced superalloys adds further complications to the numerical modeling procedure [Hopkins and Chamis (1984)] and requires an enhancement of present methods to handle such material models. The physical background of the problem is summarized in Hartman (1984), and Cook, Laflen (1984).

A literature survey by Fyhre and Hughes (1983) covers the papers and reports on finite elements potentially useful to this class of problems. The report presents a broad overview of the field rather than indicating a specific direction. The objective of this survey is more specific. After the development of new technology reported in Todd, Cassenti, Nakazawa and Banerjee (1984), efforts are now concentrated on the numerical techniques directly applicable to further enhancement of the methodology generated in this project.

3.1.2 Finite Element Approximations

This section surveys the development of spatial discretization methodology in finite elements. Historically, numerical tricks and local approximations have been introduced in the displacement finite element method. These improve the numerical performance, but do not always satisfy the variational principle. Thus, "variational crimes" originated. Then, efforts to mathematically legitimize such ad hoc schemes followed.

The variational formulation and the element technology are not clearly separable. However, to make the underlying mathematical structure visible, the following sections attempt to separately review: (1) the global variational forms, and (2) the construction of elements.

3.1.2.1 Variational Formulations

The most general form of the variational functional was constructed originally by Hu (1955) and Washizu (1955) for a class of problems in linear elasticity. The development of this principle for a range of problems in mechanics is fully documented by Washizu (1974) and Oden, Reddy (1976), and for the derivation for linear elasticity by Oden (1979). The practical importance of this form was not recognized until recently [Zienkiewicz (1977), ch. 12, page 310].

The historical development of variational calculus and the important fundamental theorems are concisely presented in Goldstein (1980). For application to the finite element method, the conceptual background can be traced back to the paper presented by Courant (1943).

Recent publications address the importance of the Hu-Washizu form and its applications. Zienkiewicz and Nakazawa (1984) discuss the equivalence of the Hu-Washizu principle and numerically integrated displacement finite element formulations. This is an important generalization of the equivalence theorem by Malkus and Hughes (1978), originally stated for a simpler class of constrained problems. Hughes and Malkus (1983) present another extension of the theorem, still in the framework of the Hellinger-Reissner principle, to a class of anisotropic and nonlinear problems.

Loubignac, Cantin, Touzot (1977) and Cantin, Loubignac, Touzot (1978) introduce a method to solve elastic problems iteratively by using continuous stress approximations. The procedure is a different manifestation of the mixed method derived from the Hellinger-Reissner principle [Zienkiewicz, Li and Nakazawa (1984)]. This procedure indeed improves the quality of the the finite element solution, in particular the stress field. A more accurate version is reported by Zienkiewicz, Vilotte, Toyoshima and Nakazawa (1984). It compares various integration schemes for the constraint equation and finds that some of them produce simultaneously super-convergent displacement and stress at nodes. The paper also points out the similarity of this procedure and the augmented

Lagrangian iteration. An extension of this procedure for a general class of inelastic problems requires the full Hu-Washizu principle. A first draft of this discussion has appeared in Todd, Cassenti, Nakazawa and Banerjee (1984) as a contract report. Construction and utilization of the augmented Hu-Washizu form and iterative solution algorithms are discussed further in Nakazawa, Nagtegaal and Zienkiewicz (1985).

An iterative cross section method proposed by Crisfield (1975) looks familiar to the algorithm discussed above. The motivation was to improve in an iterative manner the transverse shear constraint for the incompatible plate element iteratively. As later criticized by Mang and Gallagher (1978), the variational structure of this scheme is not consistent with the theory and the result is dubious. The construction of iterative solution algorithms for incompatible plates with a firm variational foundation first appeared in Todd, Cassenti, Nakazawa and Banerjee (1984). In addition, Miller and Hughes (1985) discuss a version of a consistent algorithm for structures.

Development of a generalized nonlinear version of the Hu-Washizu principle for finite strain, incompressible plasticity is reported by Simo, Taylor and Pister (1984). The principle is also extended to the formulation of finite strain viscoelasticity by Simo (1985).

The Hu-Washizu principle is used extensively as a vehicle to derive the hybrid variational principle and the hybrid finite elements. An outline of the derivation is presented in Oden and Reddy (1976). An example of the hybrid plate stiffness is given in Spilker and Belytschko (1983). The finite element formulation is similar (often identical) to the discretized plate and shell model originally derived by Reissner (1948) and Mindlin (1951). These forms relax the C^1-continuity requirement of the admissible variations and make the construction of finite elements simpler. The numerical methods derived from these principles are often called the Mindlin plate, or more properly the Reissner-Mindlin plate models.

Problems with constraints need special treatment. The constrained variational form seeks a solution in a subset in which the constraint is identically satisfied. The discretized version of this form finds a solution in an approximation subset where the constraint is also identically satisfied. The construction of such a finite element basis is not always straightforward. A number of approximation procedures have been developed for plates and shells (often referred to as the discrete Kirchhoff method) and for incompressible problems.

When inequality constraints such as contact and friction conditions are imposed on solid and structural problems, they are formulated by variational inequalities. The formulation is useful to demonstrate the mathematical complexity of this class of problems. Lions and Stampaccia (1967) present the derivation without directly referring to minimization theory. They also discuss the existence and uniqueness of a class of variational inequalities. A tutorial is prepared by Oden, Kikuchi (1977) and Kikuchi, Oden (1979), which includes a discussion on the finite element approximations of the inequality constraints. For a general class of inelastic problems, the Hu-Washizu variational formulation can be cast into a system involving an inequality and equalities. This modification appeared in Nagtegaal and Nakazawa (1985). Again difficulties are encountered when an analyst attempts to construct the approximation subset directly for this class of problems.

The mixed variational formulation and its finite element counterpart were first derived for problems with incompressibility constraints. Hermann (1965) introduces the Lagrange multiplier for the equality constraint and sets up finite element equations which include the displacement and discretized Lagrange multiplier as unknown variables. The unconstrained displacement subspace is used in this computation in conjunction with the subspace in which the multiplier lies.

The perturbed form of the Lagrangian functional satisfies the constraint approximately. The Lagrange multiplier can be eliminated from this form to produce the penalty function form. Zienkiewicz (1974) provides documentation for the motivation and a preliminary discussion on the penalty form. The variational argument for the constant dilatation element in Nagtegaal, Parks and Rice (1974) also results in the same formulation for the problem of plasticity. As discussed in Oden, Kikuchi (1982) and Kikuchi, Song (1982), the same modification is possible for problems with inequality constraints.

The elimination of the constraint in the set of admissible functions introduces a different problem related to the admissible space for the Lagrange multipliers, which looks equally if not more complicated. The difficulty is the condition for stability related to the space for the Lagrange multiplier. The continuous form satisfies the necessary condition for stability identically, but the finite element approximations do not satisfy the same condition and need special attention. This is discussed in detail in the next section.

Identification of the Lagrange multiplier by the field variable leads to a simplified (i.e., modified) variational formulation originally derived by Rudiger (1960). Its numerical solution in the form of the hybrid displacement method is reported by Kikuchi and Ando (1972), which was the subject of controversy. A general procedure is discussed in Zienkiewicz (1977) and is applied to combine the solution of the boundary and finite element procedures [Zienkiewicz, Kelly and Bettess (1979)]. Zienkiewicz and Nakazawa (1984) demonstrate the utilization of such a principle to problems with an interface. Oden and Martins (1984) applied this procedure to generate a surface force term in variational formulation for friction problems. In recent papers, Mang, Gallagher (1977, 1978), Haugeneder, Mang (1979), and Mang, Hofstetter, Gallagher (1985) repeatedly discuss the virtues and vices of this simplified form. Some of these papers are philosophical rather than technical, and the statements made therein might be discounted. The conclusions drawn in these papers are negative, and do not provide a confident basis to fully exploit the simplified form for a wide range of applications. But this does not disqualify the concept. Xue and Atluri (1985) discuss the lack of stability of this class of variational formulations. However, the result does not fully explain the successes and failures reported in the previous papers.

Instead of directly referring to the variational functional, the finite element method can be derived from the method of weighted residuals [Finlayson (1972)]. Early literature on the method discusses the virtues and vices of these two formulations [Oden (1969A,B)]. In recent years textbooks have been published which develop the finite element concept almost exclusively from the Galerkin method concept [Fairweather (1978) and Fletcher (1984)]. The slight discrepancy between these two notions is sometimes useful (but not essential) when the method is applied to non-self-adjoint problems often encountered in fluid mechanics. Examples are use of the Petrov-Galerkin methods to generate the upwinding effect for convection dominated problems [Hughes and Brooks (1979) among many others].

As discussed in the standard mathematics textbooks [Lions, Magnes (1972) and Aubin (1972)], these two different ways of telling the story (i.e., the variational functional method and the weighted residual method) are essentially slightly different manifestations of the theory of differential equations. The use of the variational method argument in which the differential equations are weighted and integrated before discretization is more useful for gaining insight into the mathematical structure of the problem and the finite element approximation process. In modern literature, the word "variational" is used almost universally, including the weak formulation for non-self adjoint problems. The word "Galerkin", which still appears in the literature, often causes confusion in communicating the mathematical reality behind the numerical methods and is to be avoided.

3.1.2.2 Element Technology

Improvement of element performance by virtue of mixed and hybrid variational formulations is currently the subject of active research. The original motivation to use these approaches was to overcome the difficulty of constructing compatible displacement finite element approximations for fourth order problems such as for Kirchhoff plates and shells. The construction of C^1-continuous elements is extremely complicated, and the resulting basis functions are prohibitively expensive to compute. Argyris, Fried and Sharpf (1968) describe one of the highest order polynomial interpolations defined on triangles and used in practical computations. An incomplete cubic triangle was developed and later documented in Zienkiewicz (1971) in which integration by the area coordinate system is introduced. This particular element satisfies the slope continuity only at the nodes, and the approximate displacement field is discontinuous over the element edge. To justify the use of a wide range of incompatible elements, the patch test was proposed by Irons (1975) and used extensively as a tool to validate new elements. Irons and Loikkanen (1983) document the recent development of this test. Taylor, Simo, Zienkiewicz and Chan (1986) attempt to develop the test for a wider range of element construction such as the mixed method. The relaxation of the slope continuity requirement by these formulations allows the use of simple C^0-continuous elements. Various techniques such as the mixed and hybrid methods have been developed for this purpose. Application of mixed and hybrid approaches has been extended beyond shell structures to include solid continua.

The development of element technology is concentrated on a simple class. The four-node quadrilateral and eight-node hexahederal elements are subjects of recent research and development. Due to the complexity of higher order interpolation functions, few if any high performance elements have emerged which use more than quadratic functions. Exceptions are work on nine-node Lagrangian shell elements which often exhibit superb numerical performance.

An extreme simplification of the approximate solution method is to use a piecewise constant displacement field as was investigated by Kawai (1978, 1980 and 1983). The method produces poor results for the displacement field, but the quality of the stress solution and the accuracy of the limit load predicted by this type of method is quite good.

Modern element technology utilizes the flexibility of the mixed and hybrid variational formulations and does not directly refer to the displacement principle. This paradigm shift legalizes "tricks" referred to as the "variational crimes" extensively used in finite element computations to increase numerical performance. The differentiation between the mixed and hybrid methods has become a subtle issue. Quite often these concepts are used to derive the stiffness equations which contain entries at precisely the same locations as the conventional displacement method. This is discussed from an historical perspective by one of the founders of the methodologies [Pian (1978 and 1983)]. A series of monographs compiled by finite element developers indeed focuses upon the development of mixed and hybrid methods including an elaborate version of the differentiation issue [Glowinski, Rodin, Zienkiewicz (1979) and Atluri, Gallagher, Zienkiewicz (1983)]. A survey has been compiled by Atluri, Tong and Murakawa (1983). In addition, progress is reviewed in a conference proceeding compiled by Spilker and Reed (1985). The name "nonstandard" finite element methods was given to this class of elements by Brezzi (1979) with a detailed mathematical analysis for fourth order equations.

For the purpose of clarity, the mixed and hybrid finite element methods are defined as:

Mixed methods -	Variational forms and finite element equations employ multiple unknown field variables which are independently interpolated. Some of these variables may be eliminated algebraically from the finite element equations.
Hybrid methods -	Constraints are introduced in the finite element forms by virtue of Lagrange multipliers defined over the inter-element boundaries. These additional terms are often eliminated from the algebraic equations resulting in a form similar to conventional displacement models. In recent publications [Pian and Chen (1982), Pian and Sumihara (1984)], the definition of hybrid methods has drastically changed. The surface integral terms are dropped from the formulation resulting in mixed stress finite elements with piecewise discontinuous interpolation for stress. Often the strain interpolation function is generated from the stress approximation under a linear isotropic elastic assumption.

The subtle issue related to this class of finite elements involves numerical stability, often referred to as the Babuska-Brezzi condition [Babuska (1973) and Brezzi (1974)]. This condition holds for the continuous problem if the solution exists. This fundamental question on mixed and hybrid finite elements was raised by Oden (1982) in the context of the penalty function formulation with selective-reduced integration for a linear, incompressible problem. The mathematical foundation of the stability issue comes from the existence theorem of variational forms often referred to as the Lax-Milgram-Babuska lemma which first appeared in Babuska and Aziz (1972).

The stability argument, as applied to constrained problems, has been addressed in many papers. Babuska, Oden and Lee (1978) introduced the stability criteria for a mixed hybrid method for linear second-order equations. For incompressible problems, Fortin (1977) studied the mathematical structure of a simple mixed formulation, e.g., bilinear displacement and piecewise constant pressure. A rate of convergence is detected in which the Babuska-Brezzi condition plays a crucial role. The analysis has been extended to include several other finite element interpolation schemes in Fortin and Thomasset (1979). A lecture by Girault and Raviart (1979) covers most of the important abstract results related to the finite element analysis of incompressible problems. Bercovier (1978) looked at the perturbed form of the mixed finite element equations and studied the role of stability condition. Oden, Jacquette (1984), Oden (1982A), Kikuchi, Oden, Song (1984), and Oden, Kikuchi, and Song (1982) discussed the necessity of finite elements having to satisfy this condition. The authors state that their results discredit popular selective integration elements such as the four-node linear and the nine-node quadratic Lagrangian bases with selectively reduced integration. From numerical experiments, a certain class of stable elements recommended by mathematicians (e.g., quadratics with single point pressure sampling) was found to be so extremely inaccurate that these elements are not usable in any practical analysis. Carey and Krishnan (1982) investigated the stability of popular penalty finite elements and redefined the stability estimates. Experimental observations are included to support the mathematical argument.

Zienkiewicz and Nakazawa (1982) demonstrate the possibility of relaxing this condition in practical computations. Similar argument can be found in Malkus and Olson (1982 and 1984). These papers strongly suggest the possibility of using popular selectively reduced integration schemes for penalty function finite elements. A proper postprocessing scheme would satisfy a posteriori the Babuska-Brezzi condition. Johnson and Pitkaranta (1982) look into the same problem and draw a positive conclusion. Kikuchi, Oden and Song (1984) propose a stable recovery scheme for unstable selectively reduced integration elements. Zienkiewicz, Taylor and Baynham (1983) introduce practical quadratic elements which satisfy the condition a priori. In the Stokes flow setting Bratianu, Atluri and Ying (1984) develop a hybrid finite element and discuss stability in the same context. This documentation insists strongly on the necessity of imposing the stability condition.

Le Tallac (1980) addresses this issue in the nonlinear elasticity setting, and proposes a patch of conventional elements which satisfies the stability condition. Glowinski and Le Tallac (1982) examined the numerical performance of popular selectively reduced integration elements. The incompressibility constraint in terms of deformation gradient for nonlinear kinematics was dealt with by the augmented Lagrangian form in these papers.

The same stability issue plays a significant role in problems with inequality constraints. Without directly using the variational inequality, binary switch algorithms for contact and friction have been developed [Francavilla and Zienkiewicz (1975)] and implemented into commercially available codes. Variational inequality was introduced to the finite element community, and a systematic effort has been mounted to study the convergence characteristics of approximate solutions for constrained problems [Glowinski (1979)]. The mixed and penalty forms of variational inequalities provide the condition for the approximation of the surface forces. Kikuchi (1982A,B) discusses the stability of the penalized form of the variational inequality and generates the classical nodally lumped nonlinear spring for contact and friction situations. In addition, a postprocessing scheme for surface force recovery is developed therein. Oden (1983) develops an approximation scheme for this class of problems. Further development of the finite element approximation for penalized variational inequalities is reported in Campos, Oden and Kikuchi (1982) including the stability considerations and smoothing algorithms.

A simple test for the stability of mixed elements similar to the classical patch test is required by engineers. There is an ongoing research effort, but a robust method has not yet been reported in the literature.

Selective and reduced integration schemes have evolved from finite element computation of plasticity. The reduced integration for continuum elements was published by Naylor (1974). A heuristic argument for a constant dilatation element, which is a four-node quadrilateral with piecewise constant pressure (i.e., one point integration), is found in Nagtegaal, Parks and Rice (1974).

The global mixed scheme, in which the additional mixed variables are interpolated continuously almost everywhere in the finite element region, has not been used extensively for obvious reasons. The original implementation of the mixed method with C^0 continuous approximations for Lagrange multipliers involves the factorization of large indefinite systems of equations [Hermann (1965 and 1967)]. The mixed approximation is also used extensively in fluid mechanics applications [Taylor, Hood (1973) and Kawahara (1978)]. As mentioned earlier, certain global mixed interpolation schemes can be used in conjunction with the equilibrium iteration algorithm. The structure of this method and a number of fully worked out examples are contained in the report [Todd, Cassenti, Nakazawa and Banerjee (1984)].

In modern literature, however, the use of piecewise discontinuous interpolation is more common than the use of globally continuous mixed interpolation. The advantage of the discontinuous mixed interpolation in conjunction with equation solution by a frontal solution algorithm is demonstrated in Nakazawa (1984).

An example of high performance continuum elements based on the hybrid stress argument has been presented by Pian and Sumihara (1984). Further development was reported in Pian and Tian (1985). A systematic approach to improve the accuracy of linear continuum elements has been presented by Belytschko and Bachrach (1985), with a discussion of the underlying variational structure discussed separately by Stolarski and Belytschko (1985). The limitation principle discussed in this paper is an extension of the concept introduced by Fraejis De Veubeke (1965).

The utilization of the Hu-Washizu principle for a class of assumed strain finite elements for plates and shells is discussed by Simo and Hughes (1985). Their argument not only extends the possible mixed finite element forms for structures but also provides a rational basis for construction of stress recovery schemes. This may potentially improve the performance of modern elements used in structural analysis such as the one proposed by Hughes and Tezduyar (1981).

It is interesting to note that the assumed strain elements have evolved from the research in selective integration techniques used for the Reissner-Mindlin plate model and the discrete Kirchhoff assumption for a class of isoparametric elements. The original papers were published as early as 1971 [Pawsey, Clough (1971) and Zienkiewicz, Taylor, Too (1971)]. A comprehensive survey has been compiled by Pugh, Hinton and Zienkiewicz (1978).

The use of under integrated elements, either by selectively reduced or by uniformly reduced quadrature, has become a common exercise in large-scale applications. A major drawback of these elements is that the resulting stiffness equations are often rank deficient. The number of zero energy modes is often larger than the number of physically meaningful rigid body modes. These additional zero energy modes are often identified as the hourglass modes for linear elements and the Escher modes for certain quadratics [Hinton and Bicanic (1979)]. When selective integration is used for the solution of incompressible problems, similar symptoms appear in terms of the approximate pressure field which is often referred to as the checkerboard pattern.

These numerical noises are mathematically identified as the extra entries in the kernel for the finite element stiffness equations. Flanagan and Belytschko (1981) identify the extra kernel vector for the four-noded linear element with one-point quadrature. This vector is then used to generate the stabilization matrix to suppress the hourglass mode. A simple scheme was developed to control the numerical noise for the selectively integrated shell elements [Belytschko, Tsay and Liu (1981)]. An extension of this procedure for the plate element with one-point quadrature is developed in Belytschko and Tsay (1983).

The same numerical instability occurs in finite difference computations, and similar hourglass control schemes have also been devised for practical computations [Maenchen and Sack (1964)].

It is insisted in Oden (1983) that the removal of the kernel a priori is not necessary since the spurious modes can be removed by a post-processing scheme. However, the factorization of a rank deficient system of equations is often impractical unless the stabilization is introduced.

3.1.3 Solution Algorithms

It has been the habit of finite element analysts to assemble the global stiffness equations and then to factorize them. The advantage of this direct solution strategy, as discussed in standard textbooks [Strang, Fix (1973) and Zienkiewicz (1977)], is the ability to obtain nodal displacements for any structure unaffected by the conditioning of the matrix with a limited and predictable amount of arithmetic operations. An often useful feature of this approach is the fact that the factor of the stiffness equations is available for different loading conditions.

For transient problems, implicit algorithms involving matrix solution have been the main vehicle for determining the nonlinear dynamic response of solids and structures. An overview is provided by Belytschko (1983), and stability behavior is discussed by Hughes (1983) in the same monograph.

The solution strategy for the stiffness equations is to utilize the sparsity and the banded structure of the coefficient matrix. Little progress has been made in the past five years except for minor refinements and improvements of existing computational procedures such as band or skyline storage (profile) solvers and frontal solution methods. In particular, a complicated, yet efficient frontal process was obtained in combination with a skyline storage scheme by Thompson and Shimazaki (1980). The skyline storage strategy is documented by Taylor in Zienkiewicz (1977) and an unsymmetric version of the frontal solution by Hood (1976), both with well-documented source programs. Also, in order to increase capacity, a partitioned storage scheme for the frontal solution has been proposed by Beer and Haas (1982). However, it is not yet clear if these types of schemes are appropriate for boosting performance in vector and/or parallel processor computers.

Interest in the iterative solution of algebraic equations was revived to enhance the capacity as well as the speed of finite element solutions. The monograph compiled by Liu, Belytschko and Park (1984) represents the state of the art of the mid-1980s. Algorithms based on the preconditioned conjugate gradient method are most commonly used for systems of well-conditioned equations. The basic theory and its application to displacement and mixed finite element equations are fully documented by Axelsson (1976 and 1978). An effort to devise a simpler preconditioner, such as the element-by-element approximate factorization, has been reported by Hughes, Winget, Levit (1983), Muller, Hughes (1984), and Muller (1985). A similar technique which uses a simpler representation of the stiffness matrix was proposed by Rashid (1969), and limited success was reported for the solution of three-dimensional problems. A comprehensive survey of these classical works on iteration is provided by Elsawaf and Irons (1982).

A construction of iterative solution algorithms for symmetric, positive definite systems of equations is discussed in an early paper by Hestens and Stiefel (1952). The conjugate gradient and preconditioned conjugate gradient procedures are used extensively for solution of finite difference equations and optimization problems.

For a class of linear problems with equality and inequality constraints, an iterative algorithm is proposed by Arrow, Hurwicz and Uzawa (1958) and referred to as Uzawa's algorithm. In this process, constraints are imposed by means of Lagrange multipliers. The algorithm has been extended independently by Hestens (1969) and Powell (1969). In comprehensive reports published by Rockafeller (1971 and 1974), the algorithm is called the augmented Lagrangian method. The basic characteristics of this scheme in a finite dimensional setting are discussed in detail by Hestens (1975).

In the finite element literature, the same concept has been developed and utilized for the solution of constrained problems such as incompressible elasticity. Applications of initial strain method in an iterative fashion are reported by Argyris (1965) and Zienkiewicz, Valliappan (1969). The penalization process and its iterative improvement are discussed by Felippa (1978) with the imposition of nodal displacement constraints as a particular example.

A comprehensive treatise on the augmented Lagrangian method in the context of finite element application has appeared [Fortin and Glowinski (1982)] in which recent developments are documented with a number of fully worked out examples.

An example of the augmented solution with nonlinear equality constraints in nonlinear elasticity is demonstrated by Le Tallac (1980). In the field of optimization, the use of iterative solutions is a lot more common than direct factorization, and the experience gained there is transferable to finite element practice. An example of such an argument is found in Kikuchi (1979). The standard textbook [Luenberger (1984)] is a useful source for potentially efficient solution schemes. In addition, a family of algorithms based on dynamic and viscous relaxation has been investigated in the modern context [Felippa (1984) and Zienkiewicz, Loehner (1983)].

The method for tracing the equilibrium path of nonlinear deformation processes in an incremental iterative fashion was developed originally by Marcal and King (1967). An incremental process to deal with the problem of plasticity by generating the tangent stiffness over an infinitesimal load step was developed by Yamada, Yoshimura and Sakurai (1968); this process is not iterative and often leads to sizable accumulation of truncation error.

The solution for incremental displacements is often constructed using Newton-Raphson iterations. This scheme requires the construction and factorization of the global Jacobian matrix for every displacement update. The modified Newton method does not need matrix assembly and solution but is a lot slower to converge. Methods based on quasi-Newton updates have started to appear in the finite element literature. Two important papers are by Matthies and Strang (1979) introducing the inverse BFGS update, and by Crisfield (1979) in which the secant Newton update is tested.

The use of the classical conjugate gradient algorithm for the solution of nonlinear solid mechanics problems was attempted with limited success by Biffle and Kreig (1981).

Application of a quasi-Newton update for fluid mechanics computations has been discussed by Engelman, Strang and Bathe (1981) in the Navier-Stokes flow setting. The Broyden update is used for nonsymmetric systems of equations. For the solution of actual problems, however, the method is combined with the traditional Newton-Raphson scheme and the direct substitution algorithm.

In these papers, it was not concluded which method is the best overall. As surveyed in Crisfield (1982), the success of schemes depends heavily on the characteristics of the specific problem being solved.

In the context of mixed iterative solution procedures, the variable metric approach was found to be more powerful than the conventional Newton-Raphson update for the problem of plasticity [Nakazawa, Nagtegaal and Zienkiewicz (1985)]. In particular, the secant Newton implementation of the Davidon rank-one quasi-Newton method was found to be the most efficient.

Automatic load adjustment schemes within the iterative displacement update have been developed to improve the performance of the nonlinear solution, in particular near bifurcation points in the equilibrium path. The algorithm originated by Riks (1979) was developed further by Crisfield (1980). A family of algorithms has also been developed to trace the complicated equilibrium path in an incremental iterative fashion [Bergan, Holand, Soreide (1979) and Bergan (1982)]. A survey is available [Crisfield (1982)] with a number of fully worked out algorithms and examples. An algorithm combining arc length and search procedures was developed by Crisfield (1983) with a limited number of examples. In addition, a series of numerical experiments has been carried out by Abdel Rhaman (1982) with detailed documentation of the algorithms.

3.1.4 Postprocessing

Numerical processes which operate on the nodal values of the finite element solution to produce information such as stresses and strains are regarded as postprocessing procedures. The definition of postprocessing and an attempt to unify the concepts involved were discussed for the first time in a systematic manner by Babuska and Miller (1984A,B,C). To obtain a smooth and potentially accurate stress field from the displacement finite element solution, a primitive form of postprocessing has been routinely performed. In fracture mechanics applications, the concept has also been used to evaluate the stress intensity factor and other quantities.

As pointed out by Melosh (1963) in the early days of finite elements, the stress values obtained by direct substitution of nodal displacement values into the stress-displacement equation are much less accurate than the displacements. Indeed, as shown in Ciarlet and Raviart (1973), the maximum error in stress values in the displacement method is a full order greater than that of displacement in terms of the L_2-norm and the maximum norm.

Schemes to calculate accurate stress fields from the given displacement solution have been the subject of intensive research. Oden and Brauchili (1971) propose use of the conjugate approximation for stress which is used as the global filtering scheme for stress. As discussed in detail by Oden and Reddy (1976), the conjugate approximation could possibly improve the quality of the finite element stress field. Theoretically, the best approximation property is expected in the mean square sense. The scheme has not gained popularity due to the expense of generating another finite element solution for the conjugate basis function. An improved computational procedure was proposed by Oden and Reddy (1973). For problems with stress concentrations for example, the global Gram matrix used to generate the conjugate basis is partitioned and the computational effort is reduced. Using the least square form of the constraint equation, a family of filtering schemes can be constructed [Hinton (1968)]. A local-global smoothing scheme for derivatives is constructed by Hinton and Campbell (1974), and its performance for eight-node quadratics has been demonstrated in Hinton, Scott, Ricketts (1975) and Zienkiewicz, Hinton (1976). The textbook by Hinton and Owen (1977) documents the details of this type of numerical procedure.

Motivated by the success of numerical filters developed for unstable pressure fields in the penalty finite element solution [Zienkiewicz, Nakazawa (1982) and Lee, Gresho, Sani (1979)], Owa (1982) investigated global stress smoothing schemes. The method, referred to as variational recovery, uses the weak variational form of the constraint equation and introduces the lumped mass approximation to generate the approximate Gram matrix. The scheme is economical since it does not involve a matrix inversion, and it is applicable to a wide range of problems without significant modification of the existing displacement finite element code [Nakazawa, Owa and Zienkiewicz (1984)]. The convergence of stress recovered by this variational process is optimal in the mean square sense as demonstrated by numerical experiments.

An algorithm to generate nodal continuous stress fields has been developed and used in an iterative solution scheme for the mixed finite element equation by Cantin, Loubignac, Touzot (1978) and Loubignac, Cantin, Touzot (1977). The numerical performance of this scheme is not satisfactory. Cook (1982) improved the quality of the stress recovery algorithm by introducing the finite difference argument on patches of regular finite elements.

Jeyachandrabose and Kinkhope (1984) propose a strain filtering scheme for the eight-node quadrilateral element. The implementation is based on a local filtering concept. The filtered strain is constructed explicitly in the matrix assembly process resulting in the so-called "assumed strain" element. In this type of algorithm, the improvement of strain convergence is only by a constant dictated by the limitation principle which states that the rate of convergence of mixed and hybrid methods in which the strain and stress are interpolated by element discontinuous functions is the same order as for the displacement method with the same displacement approximations.

3.1.5 Conclusions

A substantial body of literature on the algorithmic and computational aspects of finite elements has appeared in the past several years. This survey covered major technical papers and reports published in the present decade and a few historically important contributions published earlier. The trend in research is to fine-tune the element technology and to streamline the solution procedure. The mixed and hybrid variational formulations play a central role in both of these aspects. These techniques are capable of handling large-scale, highly nonlinear problems in engineering because of recent developments in numerical methods and the significantly improved performance of modern hardware.

Directions of future research and development, whose objective is to provide more accurate and efficient computational procedures, have become clearly visible from the literature surveyed herein. There have been, and will continue to be, two paths to take:

1. For a given finite element mesh, extract more information more accurately, and

2. For a given computer (constraint on the speed and capacity), accommodate larger meshes and crunch numbers in a feasible period of time.

The spatial and temporal approximation strategy will allow realization of the first target. As discussed in this survey, the mixed and hybrid finite element concepts have been used to derive simple and highly accurate elements for two- and three-dimensional continua and three-dimensional shells. Further work to exploit the full potential of these "nonstandard" methodologies will improve the quality of the numerical solution. In particular, the utilization of continuous functions for the derivatives of field variables, i.e., displacement gradient, strain and stress, will potentially result in a robust numerical scheme. The stability and convergence rate (if the method at all converges) are yet to be determined. The mathematical structure of the general mixed finite element approximations should be an important subject of future research. In addition, the analysis of special cases such as singularities in strain and stress and material interfaces must be treated carefully in this type of methodology. Construction of approximation techniques must include these details.

Reduction of core storage requirements and increases in speed partly rely on the element technology. The number of points where functions are evaluated is proportional to the number of arithmetic operations. Lower order integration and control of the kinematic modes associated with under-integration are crucial ingredients in the element technology. Further development and more numerical experimentation are required in this area.

A large portion of the computing time is consumed by the solution of linear algebraic equations in finite element analysis. An efficient solver is a key ingredient for overall efficiency. Iterative solvers should be investigated with particular applications to ill-conditioned problems such as those arising from the Timoshenko beam and Reissner-Mindlin shell theories. In nonlinear calculations, the Newton-Raphson process repeatedly assembles and factorizes the global stiffness equations which are the most expensive operations. Quasi- and secant-Newton processes will potentially decrease the cost of nonlinear solutions. The combination of an iterative linear equation solution together with nonlinear algorithms will be the subject of research and development in order to realize high performance software. The augmented Hu-Washizu formulation will provide a framework for the development of a family of preconditioned iteration algorithms. The key issue in this exercise is to construct a good preconditioner for the nonlinear iteration. In transient computations, the partitioned and operator splitting methods have similar characteristics, and investigations may result in an efficient finite element package. Comparison of high performance implicit schemes and explicit integrators should be made on a state-of-the-art coding basis. The recent investigations indicate that viscous and dynamic relaxation might result in an efficient solution package. This is also a subject of further evaluation.

Postprocessing is a powerful method to increase the information extracted from a given finite element mesh. The augmented Hu-Washizu argument suggests that the result could be used iteratively to improve the overall quality of the finite element solution. The error estimator and indicator developed as a part of postprocessing are useful in avoiding unnecessary mesh-refinement, leading to an economical analysis strategy. The combination of an *a posteriori* error estimate and self-adaptive mesh refinement is useful for improvement of the numerical solution. The details of implementation will continue to be a subject of research and development. Comparisons of h- and p-version refinement are to be made in the nonlinear environment. The solution method for the enriched finite element model is not trivial. Here again, potential utilization of iterative solution algorithms should play a major role. The mixed finite element concept will provide here a wider range of possible tactics to refine the mesh than the straight displacement method.

Modern computers exploit multiple processors in parallel or in vector form. Coding strategy to avoid excessive conditional jumping in loops will increase the throughput of these computers. In the equation solution phase, vectorizability and parallelizability are important points for evaluation. Not enough evidence has been accumulated to decide upon which solver is the most suitable for those machines. Currently, the machine dependency and code dependency of performance figures are unavoidable, and rationalization is required.

3.2 Global Solution Strategy and Element Technology

3.2.1 Introduction

Iterative methods are presented in this section for the solution of a class of indefinite systems of equations arising from the finite element discretization of mixed variational formulations.

The main advantage of mixed methods is explicit integration of the constraint equations, which leads to stable and accurate numerical approximations in the finite element analysis. Disadvantages of the mixed approach are mainly due to the additional (mixed) variables resulting in a larger indefinite system of algebraic equations. Attempts have been made to solve the mixed finite element equations directly, which is, however, prohibitively expensive for practical computations.

An iterative process will be constructed using the conventional displacement stiffness matrix (or its perturbed form with respect to the discretized constraint equations) as the preconditioner. A primitive version of this solution strategy was tested in Cantin, Loubignac and Touzot (1978) with application to problems of linear elasticity. The nodal continuous stress field was constructed based on the extrapolation process and was fed into the equilibrium iteration loop. The results were such that the accurate stress field was obtained, whereas the quality of the displacement solution deteriorated considerably.

3.2.2 The Augmented Hu-Washizu Formulation

Based upon the conventional virtual work statement in terms of displacement, a minimization problem of a functional is obtained:

$$I\,(\underset{\sim}{u}) = \frac{1}{2} \int_{\Omega} u_{i,j}\, D_{ijrs}\, u_{r,s}\; d\underset{\sim}{x} \qquad (1)$$

which leads to a finite element equation:

$$\underset{\sim}{K}\;\underset{\sim}{u} = \underset{\sim}{F} \qquad (2)$$

with $\underset{\sim}{K}$ being the stiffness matrix. The total number of stress/strain sampling points in a given mesh is denoted by N_g. With application to inelastic analysis of continua, a vector of length $(n^2 + n)\, N_g$, where n is the number of dimensions, is required to store the state of stress and the deformation history.

The finite element method derived from the Hu-Washizu principle is augmented by the displacement method, equation (2), resulting in:

$$\begin{bmatrix} \underset{\sim}{K} & \underset{\sim}{0} & \underset{\sim}{B} \\ \underset{\sim}{0} & \underset{\sim}{D} & -\underset{\sim}{C} \\ \underset{\sim}{B}^T & -\underset{\sim}{C}^T & \underset{\sim}{0} \end{bmatrix} \begin{Bmatrix} \underset{\sim}{u} \\ \underset{\sim}{e} \\ \underset{\sim}{s} \end{Bmatrix} = \begin{Bmatrix} \underset{\sim}{F} + \underset{\sim}{K}\,\underset{\sim}{u} \\ \underset{\sim}{0} \\ \underset{\sim}{0} \end{Bmatrix} \qquad (3)$$

and this form is used to construct the iteration algorithms.

The matrix $\underset{\sim}{B}$ is the discrete gradient operator, the integration of which is carried out in an element-by-element manner. The population is identical to the conventional strain-displacement matrix. The matrix $\underset{\sim}{C}$ represents the strain (stress) projection operator which generates nodal strain (stress) values from the displacement gradient (or the stress sample $\underset{\sim}{D}\,\underset{\sim}{B}\,\underset{\sim}{u}$) calculated at certain sampling points.

In the following algorithmic discussions, the possible interpolation functions for mixed variables are not limited to the element discontinuous polynomials. One of the advantages of the mixed method to be utilized in the present investigation is indeed utilization of continuous strain and stress approximations almost everywhere in the problem domain.

3.2.3 Iterative Algorithms

First, the implementation of Uzawa's algorithm is considered. Using the notation := to denote the assignment operator, the flowchart is:

(1) Initialize the displacement and residual vector $\underset{\sim}{u} := \underset{\sim}{0}$ and $\underset{\sim}{R} := \underset{\sim}{F}$

(2) Displacement solution by factorizing the stiffness equations $\underset{\sim}{K}\,\underset{\sim}{u} = \underset{\sim}{R}$

(3) Strain projection using the third equation in the Hu-Washizu finite element form (3) $\underset{\sim}{e} := \underset{\sim}{C}^{-T}\,\underset{\sim}{B}^T\,\underset{\sim}{u}$

(4) Stress Recovery using the second equation in the Hu-Washizu finite element form (3) $\underset{\sim}{s} := \underset{\sim}{C}^{-1}\,\underset{\sim}{D}\,\underset{\sim}{e}$

(5) Form the residual $\underset{\sim}{R} := \underset{\sim}{F} - \underset{\sim}{B}\,\underset{\sim}{s}$

(6) If convergent ($\|\underset{\sim}{R}\|$ less than the prescribed tolerance), then exit; else proceed to step (7)

(7) Displacement update by back substitution $\underset{\sim}{u} := \underset{\sim}{u} + \underset{\sim}{K}^{-1} \underset{\sim}{R}$

(8) Repeat from Step (3)

In linear elastic calculations, the computational overhead to carry out this iteration is significant in terms of the storage requirements. The stress, strain and residual arrays have to be assigned explicitly, requiring $nN_d + (n^2 + n)N_s$ more words where N_d is the number of displacement nodes and N_s is the number of stress nodes. In the above flowchart, it is assumed that the stiffness equations are factorized only once at Step (2) and that the factors reside in the memory until a new system of equations is assembled. The update in Step (7) only involves a back-substitution. The discrete gradient operator $\underset{\sim}{B}$ is formed as part of the residual recovery process, requiring additional arithmetic manipulations.

The key ingredient for economy in the iterative algorithms is to diagonalize the discrete projection operator $\underset{\sim}{C}$. Then, a vector of length N_s (instead of $N_s{}^2$) needs to be added. The same array is repeatedly used $1/2\,(n^2 + n)$ times, over the components of the strain vector.

Provided that the particular mixed scheme gives a better solution than the preconditioner, the iterative strategy can be viewed as an inexpensive tool to improve the quality of the results obtained via the displacement finite element method. The iteration loop from Steps (3) to (8) is a postprocessing operation by virtue of the strain/stress projection. The operation can be truncated at any stage, and the residual calculated from the mixed stress approximation is then utilized as an error estimator of the finite element discretization.

Line search, as incorporated in Uzawa's algorithm, seeks the new search direction by the orthogonality condition:

$$\Delta \underset{\sim}{u}\, \underset{\sim}{R}\, (\underset{\sim}{u} + \Lambda\, \Delta \underset{\sim}{u}) = 0 \tag{4}$$

where $\Delta\underset{\sim}{u}$ and $\underset{\sim}{R}(\underset{\sim}{u})$ are the iterative displacement update and the residual load vector associated with displacement $\underset{\sim}{u}$ respectively defined by:

$$\Delta \underset{\sim}{u} = \underset{\sim}{K}^{-1} \underset{\sim}{R} \quad ; \quad \underset{\sim}{R} = \underset{\sim}{F} - \underset{\sim}{B}\, \underset{\sim}{s} \tag{5}$$

and displacement is updated by:

$$\underset{\sim}{u} := \underset{\sim}{u} + \Lambda\, \Delta \underset{\sim}{u} \tag{6}$$

For linear problems, the parameter is directly calculated from a formula:

$$\Lambda = - \frac{\Delta \underset{\sim}{u}^T \underset{\sim}{R}\, (\underset{\sim}{u})}{\Delta \underset{\sim}{u}^T \underset{\sim}{B}\, \Delta \underset{\sim}{s}} \tag{7}$$

where $\Delta\underset{\sim}{s}$ is the iterative stress update associated with the displacement update $\Delta\underset{\sim}{u}$.

The algorithm referred to as the steepest descent method is described schematically as:

(1) Initialize $\underset{\sim}{u}: = \underset{\sim}{0}$ and $\underset{\sim}{R}: = \underset{\sim}{F}$

(2) Displacement solution by factorizing the displacement stiffness equation $\underset{\sim}{K}\,\underset{\sim}{u} = \underset{\sim}{R}$

(3) Strain projection $\underset{\sim}{e}: = \underset{\sim}{C}^{-T}\,\underset{\sim}{B}\,\underset{\sim}{u}$

(4) Stress recovery $\underset{\sim}{s}: = \underset{\sim}{C}^{-T}\,\underset{\sim}{D}\,\underset{\sim}{e}$

(5) Form the residual $\underset{\sim}{R}^{*}: = \underset{\sim}{F} - \underset{\sim}{B}\,\underset{\sim}{s}$

(6) If convergent ($\| R \|$ less than prescribed tolerance), then exit; else proceed to step (7)

(7) Iterative displacement update by back substitution $\Delta\,\underset{\sim}{u}: = \underset{\sim}{K}^{-1}\,\underset{\sim}{R}$

(8) Strain projection $\underset{\sim}{e}: = \underset{\sim}{C}^{T}\,B\,(\underset{\sim}{u} + \Delta\,\underset{\sim}{u})$

(9) Stress recovery $\underset{\sim}{s}: = \underset{\sim}{C}^{-T}\,\underset{\sim}{D}\,\underset{\sim}{e}$

(10) Form residual $\underset{\sim}{R}: = \underset{\sim}{F} - \underset{\sim}{B}\,\underset{\sim}{s}$

(11) Line search

$$\Lambda = \frac{\Delta\,\underset{\sim}{u}^{T}\,\underset{\sim}{R}^{*}}{\Delta\,\underset{\sim}{u}^{T}\,(\underset{\sim}{R} - \underset{\sim}{R}^{*})}$$

(12) Displacement update $\underset{\sim}{u}: = \underset{\sim}{u} + \Lambda\,\Delta\,\underset{\sim}{u}$

(13) Repeat from step (2)

The conjugate gradient is now introduced to search for the solution in a more efficient manner. In this algorithm, the directions are orthogonal with respect to the symmetric positive definite matrix appropriate for mixed finite elements. Note that the global mixed stiffness does not need to be formed explicitly. The residual vector calculated in the mixed manner is used to reflect the variational structure. The flowchart is:

(1) Initialize $\underset{\sim}{u} := \underset{\sim}{0}\ \underset{\sim}{s} := \underset{\sim}{0},\ s = 1$ and $\underset{\sim}{R} := \underset{\sim}{F}$

(2) Displacement solution $\underset{\sim}{K}\,\underset{\sim}{u} = \underset{\sim}{R}\ ;\ \Delta\,\underset{\sim}{u}^{*} := u\ ;\ \delta_0 := \underset{\sim}{u}^{T}\underset{\sim}{R}$

(3) Strain projection $\underset{\sim}{e} := \underset{\sim}{C}^{-T}\,\underset{\sim}{B}\,\underset{\sim}{u}$

(4) Stress recovery $\underset{\sim}{s} := \underset{\sim}{C}^{-1}\,\underset{\sim}{D}\,\underset{\sim}{e}$

(5) Form the residual $\underset{\sim}{R}^{*} := \underset{\sim}{F} - \underset{\sim}{B}\,\underset{\sim}{s}$

(6) If convergent ($\| R \|$ less than prescribed tolerance), then exit; else proceed to step (7)

(7) Preconditioning $\Delta\,\underset{\sim}{u} := \underset{\sim}{K}^{-1}\,\underset{\sim}{R}^{*}\ ;\ \delta_1 := \underset{\sim}{R}^{*T}\,\Delta\,\underset{\sim}{u}$

(8) Displacement update $\beta := \delta_1 / \delta_0\ ;$

$\Delta\,\underset{\sim}{u}^{*} := \Delta\,\underset{\sim}{u} + \beta\,\Delta\,\underset{\sim}{u}^{*}\ ;$

$\delta_0 := \delta_1$

(9) Line search to find the search distance s with respect to $\Delta\,\underset{\sim}{u}^{*}$

(10) Displacement update $\underset{\sim}{u} := \underset{\sim}{u} + \Lambda\,\Delta\,\underset{\sim}{u}^{*}$

(11) Repeat from step (3)

It is possible to use modern numerical methods to update the preconditioner in an effort to improve the convergence of the iterative processes. Typically, the utilization of quasi-Newton algorithms is an attractive alternative to the class of schemes discussed above.

The particular algorithm considered here is the inverse BFGS update based on the product formula:

$$\underline{K}_n^{-1} = \prod_{j=n}^{1} (1 + \underline{w}_j \, \underline{v}_j^T) \, \underline{K}_0^{-1} \prod_{k=1}^{n} (1 + \underline{v}_j \, \underline{w}_j^T) \tag{8}$$

in which the update vectors are calculated from the residual based on the mixed finite element formulation as follows:

$$\underline{v}_j = \Delta \underline{u}_j \, / \, \Delta \underline{u}_j^T \, \underline{\gamma}_j \quad , \tag{9}$$

$$\underline{w}_j = \underline{R}_{j-1} \left(1 + \left| \frac{\Delta \underline{u}_j^T \, \underline{\gamma}_j}{\Delta \underline{u}_j^T \, \underline{R}_{j-1}} \right|^{1/2} \right) - \underline{R}_j \quad . \tag{10}$$

where

$$\underline{\gamma}_j = \underline{R}_j - \underline{R}_{j-1} \quad .$$

The scheme is implemented with and without line search. Note that the summation convention is not implied in the above formulae for the subscripts representing the iteration counter.

In the computational procedure, the updated inverse replaces the inverse of the preconditioning matrix that appeared in Step (7) of the flowcharts for Uzawa's algorithm and the method of optimal descent.

In the implementation, a fixed number of update vectors is stored, typically 10, for both linear and nonlinear computations.

A variable metric alternative to the quasi-Newton method is the secant Newton procedure. The Davidon rank-one quasi-Newton update in the secant form is utilized, that is:

$$\underline{K}_n^{-1} = \underline{K}_{n-1}^{-1} + \frac{\left(\Delta \underline{u}_{n-1} - \underline{K}_{n-1}^{-1} \underline{\gamma}_n \right) \left(\Delta \underline{u}_{n-1} - \underline{K}_{n-1}^{-1} \underline{\gamma}_n \right)^T}{\left(\Delta u_{n-1} - \underline{K}_{n-1}^{-1} \gamma_n \right)^T \underline{\gamma}_n} \tag{11}$$

with n being the iteration counter, resulting in an update formula:

$$\Delta \underset{\sim}{u}_n = \bar{A} \, \Delta \underset{\sim}{u}^*_n + \bar{B} \, \Delta \underset{\sim}{u}_{n-1} + \bar{C} \, \Delta \underset{\sim}{u}^*_n \quad , \tag{12}$$

where

$$\Delta \underset{\sim}{u}^*_n = \underset{\sim}{K}_1^{-1} \, \underset{\sim}{R}_n \tag{13}$$

and

$$\bar{C} = \frac{\left(\Delta \underset{\sim}{u}_{n-1} + \Delta \underset{\sim}{u}^*_n - \Delta u^*_{n-1}\right)^T \underset{\sim}{R}_n}{\left(\Delta \underset{\sim}{u}_{n-1} + \Delta u^*_n - \Delta u^*_{n-1}\right)^T \underset{\sim}{\gamma}_n} \quad , \tag{14}$$

$$\bar{A} = 1 - \bar{C} \quad ; \quad \bar{B} = -\bar{C} \quad . \tag{15}$$

This procedure does not require the storage of update vectors. The line search operation can also be incorporated into the numerical implementation. The interaction of this update process and the mixed iteration is limited only to the replacement of the displacement preconditioning by the above formula.

It is interesting to note that, according to the author's knowledge, no attempt so far has been reported on utilizing the variable metric process for the iterative solution of linear finite element equations.

3.2.4 Nonlinear Solution Processes

Consider a quasi-static analysis of infinitesimal deformation processes. The finite element solution strategy is to subdivide the loading history into a number of successive load increments and repeat the Newton type iteration at each load level.

Algorithms developed here are to embed the mixed finite element concept in the Newton iteration. The conventional strategy of implementing iterative solution algorithms is to code a nested inner loop inside of the existing nonlinear equation solution. This strategy may be economical if the core storage requirement is reduced by the decreased population of the preconditioner, and if convergence is achieved within a reasonable number of iterations.

In the incremental processes, the role of the constitutive equation is to calculate the state of stress for a given strain increment and a strain level accumulated at the beginning of the increment. The construction of a material tangent is a computational issue, which possibly improves the displacement preconditioner in the nonlinear iterations.

The concept inherent in displacement methods which requires the constitutive equation to be identically satisfied everywhere in the domain is not necessarily compatible with the actual computational procedure when it is applied to nonlinear problems. In addition, this concept requires that the material tangent be calculated accurately everywhere in the finite element mesh. The mixed finite element concept based upon the Hu-Washizu principle describes the control structure of most finite element codes in a more straightforward and perhaps rational manner.

> The variational statement for the displacement method assumes the constitutive equation to be satisfied identically so that the strain and stress can be eliminated from the calculations. The material modulus needs to be given exactly at the state of stress and given deformation history to be able to make such elimination possible. However, inelastic material response is often given only as an implicit function of deformation history, state of stress and internal variables such as back stress. It is not feasible, even for a simple elastic-ideally-plastic material over a finite deformation increment, to derive an appropriate explicit stress expression in terms of strain and other internal variables. Thus, the constitutive relation which is to be used in the construction of the stiffness equations based on the displacement method concept can not really be exact.

The computational procedure for the state-of-the-art plasticity model is to include a subprocess to recover the stress based on the radial return concept in the iteration loop. The subprocess involves two steps:

1. Calculate the trial stress assuming the current strain increment is elastic.

2. If the process is plastic, determine the radial return direction and intersection with the yield surface and evaluate the total stress accordingly and return; or else if the process is elastic, return.

The nonlinear solution process at a given load level $\underset{\sim}{F}$ and increment $\Delta\underset{\sim}{F}$ is as follows:

(1) Initialize arrays $\quad \Delta\underset{\sim}{u}, d\underset{\sim}{u}, \Delta\underset{\sim}{\varepsilon}, \Delta\underset{\sim}{s}$ and $\underset{\sim}{R}$

(2) Construct $\quad \underset{\sim}{K}_T \, d\underset{\sim}{u} = \underset{\sim}{F} - \underset{\sim}{R}$

(3) Update $\quad \Delta\underset{\sim}{u} := \Delta\underset{\sim}{u} + d\underset{\sim}{u}$

(4) Strain recovery $\quad \Delta\underset{\sim}{\varepsilon} := \underset{\sim}{C}^{-1} \underset{\sim}{B}^T \Delta\underset{\sim}{u}$

(5) Stress recovery: Use the subprocess defined above and subtract the $\underset{\sim}{s}$ associated with the end of the previous increment to generate an incremental stress array $\Delta\underset{\sim}{s}$ associated with the current displacement increment

(6) Residual calculation $\quad \underset{\sim}{R} := \underset{\sim}{F} + \Delta\underset{\sim}{F} - \underset{\sim}{B}\,(\underset{\sim}{s} + \Delta\underset{\sim}{s})$

(7) If convergent ($\|R\|$ less than prescribed tolerance), then exit; else repeat from step (2)

The iterative solution converges when the equilibrium condition is satisfied, regardless of the quality of the tangent array $\underset{\sim}{K}_T$. Step (2) contributes to the process only as displacement preconditioning in the general nonlinear environment, even when the displacement type approach is utilized.

The preconditioned iteration algorithm developed and tested in the present status report is limited to linear and nonlinear material problems undergoing infinitesimal deformation. It is noted that for problems of finite deformation, the same iterative procedures would apply. Finite deformation kinematics related to geometry updating can be built into the stress, strain and residual recovery calculations. Such geometry updating effects will be incorporated into the MHOST code in conjunction with the large displacement option to be developed during the fourth year of contract work. In the framework of the displacement finite element method, application of a preconditioned iterative solution without explicit recalculation of the stiffness matrix has been demonstrated by Crisfield (1980, 1982). Examples discussed in these references include bifurcation due to geometrical nonlinearity among others.

It is interesting to note that the preconditioned iteration algorithm is similar to the Newton-Raphson algorithm commonly used for standard nonlinear finite element computations except for the variational recovery of nodal strain. In the Newton-Raphson algorithm, as applied to finite deformation processes involving geometry updating, the approximate tangent stiffness matrix is generated with respect to the configuration given by the last displacement update. The displacement vector is updated using this tangent stiffness matrix. Then the strain and stress recovery calculation is performed in the usual manner in which finite deformation kinematics is taken into account. The iteration continues until the residual vector becomes almost equal to the external force vector in the deformed configuration. It can be strongly argued that the consistently updated tangent stiffness matrix improves the convergence characteristics of the iterative process. However, as the algebra indicates, the final solution obtained by Newton-Raphson-like methods is governed only by the equilibrium condition with respect to the approximate stress field, regardless of the stiffness matrix update in the nonlinear calculations.

The advantage of the Newton-Raphson method in which the tangent stiffness matrix is assembled taking the geometry update into account is that sometimes it converges in fewer iterations than other Newton-Raphson-like methods because the quality of the approximated stiffness matrix is somewhat better than those updated by algebraic means in the BFGS and secant Newton methods. However, it is questionable if the additional expense of reformulating the stiffness and factorizing it is justifiable for large three-dimensional computations.

In comparison with the Newton-Raphson method, as briefly discussed above, the preconditioned iteration algorithms described in this status report are generally more economical than the method involving repeated stiffness matrix assembly and factorization at each iteration. The change in the residual vector contains sufficient information to update algebraically the tangent array or its factors and such an approach is used in the quasi-Newton algorithms implemented in the MHOST code.

In medium to large-scale finite element computations, the cost of stress recovery is often comparable in order of magnitude to the factorization of the tangent stiffness matrix. It is often possible to save on computing costs by choosing an appropriate basis for the stress interpolation so that N_s is less than N_g.

As discussed in the previous section, the numerical performance of the nonlinear solution is improved by introducing several numerical ingredients. Indeed the methods of quasi- and secant-Newton were originally developed to solve nonlinear systems of equations.

Major operations in the iterative process are the update procedure of $\underset{\sim}{K}_T$ used in Step (2) and the displacement update in Step (3). An alternative to the modified-, quasi- and secant-Newton processes, for nonlinear problems is the Newton-Raphson update, which involves assembling and factorizing the tangent stiffness array at every iteration cycle. This method is not a particularly attractive option unless a $\underset{\sim}{K}_T$ identical to the mixed stiffness matrix could explicitly be calculated. The line search is also not an attractive option since multiple evaluations of the stress factor are required.

Use of the arc-length method to control simultaneously the incremental load level and the iterative process is a useful option in conjunction with the modified-Newton, constant metric method. Exactly the same procedure as the displacement type is usable and is expressed schematically by the following flowchart:

(1) Set the residual vector R: = 0, initialize the incremental displacement vector Δu: = 0. If the first increment, initialize the total load factor λ.

(2) Project the displacement by

$$d\underset{\sim}{u} := \underset{\sim}{K}_T^{-1} \underset{\sim}{F}$$

and if it is the first cycle of iteration, calculate the arc length and initialize the incremental load factor $\Delta\lambda$ and $d\lambda$. Then, calculate the correction vector.

$$d\underset{\sim}{u} := \underset{\sim}{K}_T^{-1} (\lambda \underset{\sim}{F} - \underset{\sim}{R})$$

(3) Update the displacement vector

$$\Delta\underset{\sim}{u} := \Delta\underset{\sim}{u} + d\underset{\sim}{\bar{u}} + d\lambda\, d\underset{\sim}{u}$$

(4) Find the total load factor update

$$\lambda := \lambda + d\lambda$$

and the incremental load factor

$$\Delta\lambda := \Delta\lambda + d\lambda$$

based on the spherical path formulation.

(5) Form the residual in the mixed manner and then check the convergence. If convergent, start the next increment, or else repeat from step (2).

3.2.5 Element Technology

3.2.5.1 Element Integration Procedures

Linear and quadratic Lagrangian elements are included in the MHOST element library. A number of different integration schemes are implemented in the numerical solution procedures. The data base for the finite element model is constructed on a nodal basis with the exception of distributed loads which are stored in the element array.

To achieve stability and coarse mesh accuracy in the mixed finite element solution, not all the terms in the equations are integrated at nodes. For the evaluation of the stiffness coefficients and the internal force vector, two-point Gaussian quadrature is used for linear elements and three-point quadrature for quadratics in each coordinate direction. A nodal quadrature (element discontinuous trapezoidal integration) is used for the strain recovery operations. All the stress components are evaluated at the global nodes.

To extract near optimal numerical performance of the elements implemented in the MHOST code, the shear strain components are evaluated at the internal element centroid.

All the integration procedures are internal operations designed to generate an accurate finite element solution and are invisible to the users as results are reported primarily at the nodal points.

3.2.5.2 Coordinate Transformations

The coordinate transformation process used for the selective integration scheme has been modified to improve the performance of the bilinear Lagrangian elements used in MHOST. In particular, the polar decomposition for two-dimensional elements has been rewritten using the simple Cayley-Hamilton formula.

For the two-dimensional Jacobian matrix $\underset{\sim}{J}$, the polar decomposition:

$$\underset{\sim}{J} = (\underset{\sim}{ROT})\ \underset{\sim}{U} \tag{16}$$

can be found from

$$\underset{\sim}{U}^2 - I_1(\underset{\sim}{U})\ \underset{\sim}{U} + I_2(\underset{\sim}{U})\ \underset{\sim}{I} = \underset{\sim}{0} \tag{17}$$

where $\underset{\sim}{U}^2 = U^t\ U$ and $\underset{\sim}{I}$ is the unit tensor. Noting that

where $\underset{\sim}{U}^2 = U^t\ U$ and $\underset{\sim}{I}$ is the unit tensor. Noting that

$$(\underset{\sim}{CH}) = \underset{\sim}{J}^T\ \underset{\sim}{J} = \underset{\sim}{U}^2 \tag{18}$$

where $\underset{\sim}{U}^2 = \underset{\sim}{U}^T \underset{\sim}{U}$

and, hence,

$$\det(\underset{\sim}{CH}) = (\det \underset{\sim}{U}^2) \tag{19}$$

the following is obtained

$$(\underset{\sim}{CH}) - I_1(\underset{\sim}{U})\, \underset{\sim}{U} + I_2(\underset{\sim}{U})\, \underset{\sim}{I} = \underset{\sim}{0} \tag{20}$$

Thus,

$$\underset{\sim}{U} = \left(I_1(\underset{\sim}{CH}) + 2\sqrt{I_2(\underset{\sim}{CH})}\right)^{-1/2} \left(\underset{\sim}{CH} + \sqrt{I_2(\underset{\sim}{CH})}\, \underset{\sim}{I}\right) \tag{21}$$

This formula can be coded in an extremely simple manner. In addition, this approach is easily extendable to three-dimensional cases/

3.3 Local Analysis Procedures

3.3.1 Introduction

This section discusses numerical solution procedures specifically designed for structures with embedded discontinuities such as holes and cracks. Two methods have been proposed and analyzed in the framework of the mixed iterative finite element solution. Both methods utilize the enriched space of strain approximations in the discretized Hu-Washizu variational formulation. The first method refines the mesh locally within the conventional finite element context and extracts information by performing an independent solution. This method is referred to as the subelement scheme. The second method includes singular functions in the strain expansions around pre-assigned singular points such as a stationary crack tip. This method is called the special function approach.

The subelement refinement strategy enhances the finite element approximations by subdividing the global elements used in the global analysis. The compatibility of the subelement displacement field with the global displacement field is maintained only at global nodal points in the local-global iteration. A series of numerical tests is conducted which includes a linear-stress patch test to validate the concept. Both linear and quadratic Lagrangian elements have been introduced for subelement computations. However, the validation effort is concentrated on linear subelement schemes including a number of problems involving large stress concentrations. A limited number of numerical experiments utilizing quadratic subelements has also been conducted.

In subelement regions, all spatially varying functions such as temperature and material properties are interpolated by the same shape functions as those used for the displacement field. When quadratics are used for subelement computations, the nodal values of the global element are interpolated quadratically. In the solution process here, the algorithm also generates quadratic fields internally for strain, stress and material moduli.

The theoretical development of the special function approach is summarized in the next subsection. In the following, the form of the regular finite element shape functions is left unspecified. The derivation is general enough to allow incorporation of these results with all mixed element types implemented in the MHOST program.

In the special function development, the singular functions are introduced only to represent strain and stress fields. For the region in which special functions are invoked, other variables such as coordinates, displacements, temperatures and material properties are interpolated by the global regular finite element shape functions.

A discussion of the subelement method is provided in the previous Annual Report (NASA CR-175060). A description of the development of the special function finite element method follows.

The dimension of the displacement approximation subspace remains unchanged, and the additional computational resources required for structural analysis with embedded discontinuities are kept insignificant in comparison with standard displacement procedures. Examples included in this report demonstrate the validity and numerical performance of the proposed procedures.

3.3.2 Crack Tip Singularity and Special Function Expansion

In the vicinity of a crack tip, the finite energy assumption leads to a hypothesis on the behavior of strain energy W, that is

$$W = \sigma_{ij}\,\varepsilon_{ij} \longrightarrow F(\theta)/r \quad \text{as} \quad r \longrightarrow 0 \tag{22}$$

under the infinitesimal deformation framework, with $\underset{\sim}{\sigma}$ and $\underset{\sim}{\varepsilon}$ denoting the stress and strain tensors respectively. In equation (22), function $F(\theta)$ is a non-singular function depending on the behavior of the structure.

For a linear elastic material, the linear relation of stress and strain implies that:

$$\sigma_{ij} \longrightarrow F_{ij}(\theta)\; r^{-1/2} \tag{23A}$$

and

$$\varepsilon_{ij} \longrightarrow G_{ij}(\theta)\; r^{-1/2} \tag{23B}$$

The behavior of an elastic-perfectly plastic material can be written as:

$$\varepsilon_{r\theta} \longrightarrow F(\theta)\, r^{-1} \tag{24}$$

with the asymptotic behavior of individual stress components being potentially well above the yield level, whereas the asymptotic behavior of the Mises stress itself takes the yield value.

When the strain-hardening of the elastic-plastic material is described by a power-law model, the stress and strain exhibit Hutchinson-Rice-Rosengren (HRR) singularities [Hutchinson (1968), Rice and Rosengren (1967)], i.e.,

$$\varepsilon_{ij} \longrightarrow F_{ij}(\theta)\, r^{-\frac{1}{N+1}} \tag{25}$$

and

$$\sigma_{ij} \longrightarrow G_{ij}(\theta)\, r^{-\frac{N}{N+1}} \tag{26}$$

where F_{ij} and G_{ij} are nonsingular tensor functions characterizing the effect of global deformation. The HRR form of the singularities contains the linear elastic and perfectly plastic material response as subclasses.

Introducing singular behavior in the strain and stress fields, the following is obtained:

$$\varepsilon_{ij} = \varepsilon_{ij}^{R} + \varepsilon_{ij}^{S} = \varepsilon_{ij}^{R} + G_{ij}(\theta)\, r^{-p} \tag{26A}$$

and

$$\sigma_{ij} = \sigma_{ij}^{R} + \sigma_{ij}^{S} = \sigma_{ij}^{R} + F_{ij}(\theta)\, r^{-q} \tag{26B}$$

where the superscripts R and S denote the regular and singular parts of the strain and stress respectively. Note that the condition:

$$p + q = 1 \tag{27}$$

is necessary to satisfy the finite energy requirement.

Now consider the displacement field. The fact that the derivatives of displacement contain a singularity does not imply that the function itself is singular. Therefore, the following local statement is valid:

$$\varepsilon_{ij} = \varepsilon^{R}_{ij} + \varepsilon^{S}_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{28}$$

If the virtual stress $\delta\underset{\sim}{\sigma}$ is decomposed as:

$$\delta\underset{\sim}{\sigma} = \delta\underset{\sim}{\sigma}^{R} + \delta\underset{\sim}{\sigma}^{S} \tag{29}$$

the global displacement gradient strain expression is constructed as:

$$\int_{\Omega} \delta\sigma_{ij}\,[\varepsilon_{ij} - \frac{1}{2}(u_{i,j} + u_{j,i})]\,d\underset{\sim}{x} = 0, \tag{30}$$

where Ω is the problem domain.

Substitution of equations (26) and (29) into (30) results in:

$$\begin{aligned}
&\int_{\Omega}(\delta\sigma^{R}_{ij}\,\varepsilon^{R}_{ij} + \delta\sigma^{R}_{ij}\,\varepsilon^{S}_{ij} + \delta\sigma^{S}_{ij}\,\varepsilon^{R}_{ij} + \delta\sigma^{S}_{ij}\,\varepsilon^{S}_{ij})\,d\underset{\sim}{x} \\
&- \frac{1}{2}\int_{\Omega} \delta\sigma^{R}_{ij}\,(u_{i,j} + u_{j,i})\,d\underset{\sim}{x} \\
&- \frac{1}{2}\int_{\Omega} \delta\sigma^{S}_{ij}\,(u_{i,j} + u_{j,i})\,d\underset{\sim}{x} \\
&= 0.
\end{aligned} \tag{31}$$

The finite element process has been derived for the weak form of the strain-displacement equation (30).

The regular terms of the strain and stress tensors are expanded by the nodal shape functions $\underset{\sim}{M}$ (same form as the displacement shape functions) as follows:

$$\sigma^{R}_{ij} = M_K\,\sigma^{R}_{ijK}\quad,\quad \varepsilon^{R}_{ij} = M_K\,\varepsilon^{R}_{ijK}, \tag{32}$$

where the uppercase subscripts are used for the nodal indices. Introducing the nodeless variable set representing the intensity of the singularity, i.e., $\underset{\sim}{\epsilon}^S$ and $\underset{\sim}{\sigma}^S$, the singular terms are approximated by:

$$\begin{aligned} \sigma_{ij}^S &= r^{-q} F_{ij}(\theta) = r^{-q} M_K^*(\theta)\, \sigma_{ijK}^S \\ \epsilon_{ij}^S &= r^{-p} \ddot{u}_{ij}(\theta) = r^{-p} M_K^*(\theta)\, \epsilon_{ijK}^S \end{aligned} \tag{33}$$

Substituting equations (32) and (33) to (31), the following matrix equation is obtained:

$$\begin{bmatrix} \underset{\sim}{C}_{RR}^* & \underset{\sim}{C}_{RS}^* \\ \underset{\sim}{C}_{SR}^* & \underset{\sim}{C}_{SS}^* \end{bmatrix} \begin{Bmatrix} \underset{\sim}{\epsilon}^R \\ \underset{\sim}{\epsilon}^S \end{Bmatrix} = \begin{Bmatrix} \underset{\sim}{B}^R & \underset{\sim}{u} \\ \underset{\sim}{B}^S & \underset{\sim}{u} \end{Bmatrix} \tag{34}$$

where

$$\underset{\sim}{C}_{RR}^* = \int_\Omega \underset{\sim}{M}^T \underset{\sim}{M}\, d\underset{\sim}{x} \tag{35}$$

$$\underset{\sim}{C}_{RS}^* = \int_\Omega (r^{-p})\, \underset{\sim}{M}^T \underset{\sim}{M}^*\, d\underset{\sim}{x} \tag{36}$$

$$\underset{\sim}{C}_{SR}^* = \int_\Omega (r^{-q})\, \underset{\sim}{M}^{*T} \underset{\sim}{M}\, d\underset{\sim}{x} \tag{37}$$

$$\underset{\sim}{C}_{SS}^* = \int_\Omega (r^{-1})\, \underset{\sim}{M}^{*T} \underset{\sim}{M}^*\, d\underset{\sim}{x} \tag{38}$$

$$\underset{\sim}{B}^R = \int_\Omega \underset{\sim}{M}^T (\nabla \underset{\sim}{N})\, d\underset{\sim}{x} \tag{39}$$

and

$$\underset{\sim}{B}^S = \int_\Omega (r^{-q})\, \underset{\sim}{M}^{*T} (\nabla \underset{\sim}{N})\, d\underset{\sim}{x} \tag{40}$$

with $\underset{\sim}{N}$ being the nodal interpolation function for the displacement.

Except for the case of linear elasticity and small-scale yielding in the vicinity of the crack tip, p = q = 1/2 does not hold, and the resulting coefficient matrix (the singular strain projection operator) is nonsymmetric. To extract the information associated with the singular behavior of the structure, the lumping technique cannot be used, and the full projection operation is inverted at the element level.

The stress recovery process is now considered. Symbolically, the local stress-strain law is written in an incremental form as follows:

$$\underset{\sim}{\dot{\sigma}} = \underset{\sim}{D}\,\underset{\sim}{\dot{\varepsilon}} \tag{41}$$

For a linear elastic material, this expression automatically yields the proper singular stress form, equation (26), with:

$$\underset{\sim}{\sigma}^R = \underset{\sim}{D}\,\underset{\sim}{\varepsilon}^R \quad ; \quad \underset{\sim}{\sigma}^S = r^{-1/2}\,\underset{\sim}{D}\,\underset{\sim}{G}(\theta) \tag{42}$$

For the more general case of a nonlinear stress-strain relationship, equation (41) is used in an incremental manner. Although the order of singularity for stress and strain can differ, the incrementally linear approach will still produce the desired singularity effects. This is because the stiffness matrix D used to relate stress and strain increments is determined by previous deformation and stress histories and thus contains the proper effects to maintain the required stress and strain singularity orders.

For a power law hardening material, equations (25) and (26), the general stress-strain relationship takes the form:

$$\sigma = \gamma\varepsilon^N \quad ; \tag{43}$$

Here, a strain singularity of order (1/N+1) in r automatically generates a singularity of order (N/N+1) in stress. It is also interesting to note that for a perfectly plastic material, N=0 and p=1, q=0; while for a linear elastic material, N=1 and p=q=1/2.

The above observations indicate that the conventional incremental stress recovery routine can be used at every point in the finite element domain. The proper singular strain input produces the proper singular stress field without directly referring to the singular stress interpolation functions.

The remaining task here is to actually construct the interpolation functions. The regular part of the finite element strain expansion is given by the linear Lagrangian basis, typically in two dimensions:

$$N_i = \frac{1}{4}\,(1 + \xi_i\,\xi)\,(1 + \eta_i\,\eta) \tag{44}$$

where ξ_i and η_i ($i = 1,2,3,4$) are the corner coordinates of a bi-square in the isoparametric plane. For the problems without singular points, the regular strain interpolations associated with the mixed finite element approach accurately approximate the field far better than the conventional displacement method.

To introduce the singular terms into the finite element expansion of the strain field, the singular point is first preassigned at a corner of the quadrilateral element. The radial coordinate associated with a singular point assigned to the i^{th} nodal point is represented in terms of the element isoparametric coordinates by:

$$r^2 = (\xi - \xi_i)^2 + (\eta - \eta_i)^2 \quad , \tag{45}$$

while the tangential direction is given by:

$$\theta = \tan^{-1} \left\{ (\eta - \eta_i) \,/\, (\xi - \xi_i) \right\} \quad , \tag{46}$$

also in the isoparametric coordinate system. Then, the singular shape functions are defined as:

$$\begin{aligned} M_j^* &= (8/\pi^2)\,(\pi/2 - \theta)\,(\pi/4 - \theta) \\ M_k^* &= (4/\pi^2)\,\theta\,(\pi/2 - \theta) \\ M_l^* &= (8/\pi^2)\,\theta\,(\theta - \pi/4) \end{aligned} \tag{47}$$

for $j=i+1$, $k=j+1$, $\ell=k+1$ and $j=j-4$
if $j>4$, $k=k-4$ if $k>4$, $\ell=\ell-4$ if $\ell>4$.

3.3.3 Coding Strategy

The singular strain function is introduced in the element strain calculation subprogram at the preassigned points as input data. No global smoothing will be carried out on the singular terms. The additional singular functions are generic and usable for both global and subelement solutions.

The effect of the singular stress field can then be evaluated when the residual vector is recovered from the finite element stress solution. The stress recovery subprogram is executed for every element with preassigned singular points.

3.4 Computer Code Development and Validation

3.4.1 Introduction

In this section, the new options added to the MHOST finite element program during Task IVB are summarized. The number of algorithmic options has increased by including several alternative iterative solution methods and the optional frontal solution subsystem. The analysis options have been enhanced to include a composite laminate data reader and direct input capability for anisotropic elastic material properties. Internally, the control structure of the code, the common blocks and the finite element data base have been revised mainly to make the code more readable and debuggable.

All the development work has been carried out on a PRIME 9955 at MARC Analysis Research Corporation. Procedures have been developed to create and test versions in the VAX/VMS, IBM/CMS and CRAY/COS environments. These procedures are executed when the installations at United Technologies Corporation/Pratt & Whitney and NASA-Lewis Research Center take place. The conversion takes typically one to two weeks including the testing.

All the codes are compiled using FORTRAN-77 compilers. However, most of the source program is compatible with the previous FORTRAN standard.

3.4.2 Solution Capabilities

Version 3.2 of the MHOST program, which is the development version used in the Task IV computer program development effort, currently supports the following options and a limited number of linear and quadratic finite elements. All of the elements are usable in a fully mixed iterative manner, but the quadratic elements may only be employed in subelement regions. The conventional displacement solution algorithm is provided as a useful option with the default being the mixed iterative method.

The programming effort is briefly summarized with regard to the control parameter keywords in alphabetical order:

*ANISOTROPY

The anisotropic material property option is flagged by this parameter. The orientation vector for the material axis must be added in the model data section. The material properties along the material axis must be given by either the *DMATRIX option (for the continuum elements, type 3, 7, 10 and 11) or *LAMINATE option (for the shell element type 75). The anisotropic plastic response of a material is described by the user subroutine ANPLAS as documented in the MHOST Users' Manual.

*BFGS

The inverse BFGS update procedure is invoked by flagging this option parameter with the default iterative algorithm being the straightforward Newton-Raphson scheme.

*BOUNDARY

The nodal displacement constraints are imposed using a penalty approach.

*BUCKLE

The initial stress matrix is formed, and an eigenvalue extraction is performed to obtain buckling modes. This option can be invoked at an arbitrary step of the incremental nonlinear solution process so as to detect the change in the buckling load due to inelastic response of the structure.

*COMPOSITE

This parameter data line invokes the composite laminate analysis option for shell element type 75. This option resets the element parameters. The number of integration layers is reduced to one, and all the components of stress resultant are used as nodal variables. In the model data section, the user has to supply all the components of the nodal force-deformation matrix by invoking the laminate option.

*CONJUGATE-GRADIENT

The conjugate gradient method is invoked by adding this parameter. The line search option is automatically turned on. Note that this option cannot be used with other iterative algorithms such as the BFGS and secant Newton-methods.

*CONSTITUTIVE

Three different constitutive formulations are included in the code for describing material behavior. They involve secant elasticity (simplified plasticity) in which the material tangent is generated for use with Newton-Raphson type iterative algorithms, von Mises plasticity with the associated flow rule treated by using the radial return algorithm, and the nonlinear viscoplastic model developed by Walker, in which an initial stress iteration using the elastic stiffness is utilized. A linear elasticity option can be flagged for experimental purposes, and the default is the conventional von Mises plasticity model. Anisotropic plasticity is invoked by updating the user subroutine ANPLAS. The dummy subroutine supplied with the MHOST code is always required to produce correct results for isotropic cases.

*CREEP

Creep effects are taken into account by integrating the time history in an explicit manner. An optional self-adaptive time step size control algorithm is also available.

*DISPLACEMENTMETHOD

This option invokes the conventional displacement model in which the residual load is evaluated directly at the integration points. In the residual calculation procedure, the element strain is calculated directly from the nodal displacements via the element strain-displacement matrix. Then the element stress is obtained as a product of the element strain and the stress-strain matrix defined at nodes and interpolated to the integration points. This operation is consistent with the formulation of displacement stiffness equations and no residual force is generated in the equilibrium iteration.

For the linear elastic stress analysis, no iteration would take place when this option is flagged. In inelastic analyses, the material tangent is interpolated and multiplied by the integration point strain which is directly sampled at the quadrature point. This option cannot be used for the advanced constitutive model since the correct material tangent is not generated.

*DISTRIBUTELOAD

Body force and surface traction loadings are referred to as distributed loads in the MHOST program. The body force option includes gravity acceleration definable in any direction and centrifugal loading with the centerline and angular velocity specified by the user. The detailed description is available in the MHOST User's Manual.

*DUPLICATENODE

The continuity of stresses at nodal points can be broken by defining two nodal points at the same geometrical location and connecting them by this option which enforces compatibility of displacements only. This option is used to define the connections between generic modeling regions.

*DYNAMIC

The generalized Newmark solution algorithm is entered by setting this flag. A simple adaptive time stepping algorithm is employed at the user's option.

*ELEMENTS

The elements included in this version of the code are described in Table I. Core allocation is performed for the nodal and element-quantities on the basis of maximum storage space requirements among the types of elements specified in this option. All the element types must be specified here including those only appearing in the subelement regions.

The element type, ITYPE, is chosen to avoid possible semantics conflicts with the MARC finite element code in which element type identification numbers 1 to 98 have already been designated to various solid, structural and heat transfer elements. For instance, the four node shell element with 6 dof (degrees-of-freedom) per node based on the Reissner-Mindlin theory is referred to as element type 75 in both MARC and MHOST. Also the two node Timoshenko beam element is referred to as type 98 in both codes. Nine-noded quadratic elements are rarely used in commercial codes, and thus these types of elements are designated as types 101, 102 and 103 in the MHOST code. Element type identification numbers over 100 are unlikely to be used in general purpose packages, and thus no conflicts are anticipated.

The parameters defined in the table are used for core allocation purposes and do not necessarily correspond to physical reality. For instance seven words are reserved to define the nodal coordinate data of shell element type 75 by NELCRD. The first three words are used for the nodal point location in the global rectangular Cartesian coordinate system and the next three words are reserved for the components of the unit normal vector on the shell surface (at the node) generated internally. The seventh word is used to store the thickness of the shell at the node.

The number of stress components stored for shell element type 75 specified by NELSTR consists of the generalized stress components preintegrated through the thickness including the in-plane twist component.

The number of material property data entries NELCHR indicates how many values are needed in the *PROPERTY model data block. Enough entries are allocated to store linear isotropic elastic constants, density and thermal expansion coefficient. To specify more complicated material response such as elastoplasticity and/or anisotropic elasticity, other parameter data lines must be added which invoke memory allocation for additional material data storage.

The index for implementing the appropriate constitutive equation, JLAW, is used to tell the program exactly which stress and strain components need be considered as well as to select the form of the matrix which relates the stress and strain components. Other internal flags are used to specify the optional nonlinear constitutive models.

Further discussion of these parameters, as well as the definition of other element characteristics, can be found in Section G of the MHOST User's Manual.

Table I

MHOST Code, Version 3.2 Elements and Parameters

	Beam	P.Stress	P.Strain	Axsym.	Brick	Shell
ITYPE	98	3 / 101	11/ 102	10/ 103	7	75
NELCRD	3	2	2	2	3	7
NELNFR	3	2	2	2	3	6
NELNOD	2	4 / 9	4 / 9	4 / 9	8	4
NELSTR	1	3	4	4	6	9
NELCHR	3	5	5	5	5	5
NELINT	2	4 / 9	4 / 9	4 / 9	8	4
NELLV	3	3	3	3	3	4
NELLAY	0	1	1	1	1	5
NDI	1	2	3	3	3	2
NSHEAR	0	1	1	1	3	3
JLAW	1	2	3	4	5	6

NELCRD	Number of coordinate data per node.
NELNFR	Number of degrees-of-freedom per node.
NELNOD	Number of nodes per element.
NELSTR	Number of stress and strain components per node.
NELCHR	Number of material property data for the element.
NELINT	Number of 'full' integration points per element.
NELLV	Number of distributed load types per element.
NELLAY	Number of layers of integration through the thickness of the shell element.
NDI	Number of direct stress components.
NSHEAR	Number of shear stress components.
JLAW	Type of the constitutive equation.

*EMBED

The subelement iteration technology is flagged by this option which signals the code to allocate the working storage for the subelement data in a hierarchical manner. The actual subelement mesh definition and the nodal- and element-data storage allocation take place when the individual subelements are defined.

*FORCES

Concentrated nodal forces are defined and stored in a incremental manner. Core allocation takes place only when this option is invoked.

*FRONTALSOLUTION

The frontal solution option for the quasi-static analysis is implemented in this version of the code. Out-of-core storage devices are utilized and, hence, capacity of the program is increased significantly.

*GMRS

Generic modeling regions are defined as collections of elements that model geometrically parametrized parts of hot section components. Multiple generic modeling regions in a given mesh are connected using the duplicate node option. Different parameters are specified for each generic modeling region, and the input data can be prepared separately. Internally, the complex of the generic modeling regions is treated as a single mesh for the purpose of constructing and solving the finite element equations. A table is prepared to report results separately for each generic modeling region.

*LINE-SEARCH

The line search option requires positive action by the user to turn it on. This algorithm may be used in conjunction with all the iteration algorithms available in the MHOST program. When the conjugate gradient iteration is used, the program automatically turns on the line search.

*LOUBIGNAC

Parameters for the numerical quadrature used in the mixed iterative processes are defined in a very precise way. Full integration, selective integration, or selective integration with filtering can be chosen for construction of the stiffness matrix. For residual vector integration, full and reduced integration can be selected. The strain integration can be performed either by using uniformly reduced integration, trapezoidal integration with the reduced shear strain approximation or the previous quadrature with the filtering option. There are three parameters for this option to select integration schemes as summarized below:

Parameter 1:	1.	Reduced integration for stress recovery
	2.	Full integration for stress recovery
	3.	(Default) Trapezoidal rule for stress recovery
Parameter 2:	1.	(Default) Full integration for residual force calculation
	2.	Reduced integration for residual force calculation
Parameter 3:	1.	Full integration for stiffness matrix assembly
	2.	Selective integration for stiffness matrix assembly
	3.	(Default) Selective integration with element Cartesian coordinate transformation for stiffness matrix assembly.

*LOUBIGNAC 3 1 3 is the system default and recommended for most of the applications.

*MODAL

The free vibration modes for linear elastic structures are extracted when this option is invoked. The subspace iteration technique is utilized, and a power shift option is included.

*NODES

All the variables are defined and reported at nodal points. In the incremental processes, deformation and stress histories are integrated and stored only at the nodal points. Note that this architecture economizes storage substantially compared with fully integrated finite element displacement methods.

*NOECHO

This option suppresses the echo print of the model data.

*OPTIMIZE

A bandwidth optimization based on the Cuthill-McGee algorithm is applicable to in-core solution processes. No optimization is available for the frontal solver.

*PERIODICLOADING

For transient calculations, nodal displacements and concentrated forces can be input as sinusoidal functions using this option.

*POST

The postprocessing file which contains all the information supplied to and generated by the code are written to FORTRAN unit number 19. This file is formatted and can easily be manipulated by commercially available postprocessing packages with minor modifications. The header record of the file is designed to be compatible with the MARC post file which is processed by many finite element graphics packages.

All the displacement and reaction force components written on the postprocessing file are in the global Cartesian coordinate system. When the user specifies nodal coordinate transformation, the displacement is printed in the user-specified coordinate system on the lineprinter output. Then the results are transformed internally to the global system before generating the postprocessing file. The postprocessing program package does not need to be told to recognize the user-specified coordinate transformation.

*PRINTSETS

The report generation is carried out on a nodal point basis with element integration point options provided by interpolation using the shape function.

*REPORT

The frequency of the line printer report generation is now controlled by this option. The default is to print at every increment.

*RESTART

This option tells MHOST to read the restart tape and set up the system to resume an analysis from the point where the tape is written.

*SCHEME

Parameters that control the characteristics of the time integration operator are definable by the user. The default is the average acceleration algorithm commonly used in nonlinear dynamic finite element analysis.

*SECANT-NEWTON

This parameter activates the secant-Newton implementation of the Davidon rank-one quasi-Newton algorithm. The core-storage requirement for this procedure is significantly less than that for the BFGS update, and execution is relatively fast. This option is recommended for inelastic analyses of solid-continua.

*STRESS

Boundary conditions for stress can be specified by the user as an option, although no mathematical justification is yet available for this type of constraint. Any stress component can be prescribed at any nodal point. Simple numerical tests have shown that inconsistent imposition of stress boundary conditions can lead to rapid divergence in the iterative process.

*TANGENT

This option invokes the modified-Newton iteration procedure. The tangent matrix is updated until a user-specified iteration count greater than or equal to one is met. No updating occurs in subsequent iterations. The default iteration count is equal to one, and the procedure generated by this value is known as the K_{T1} method of modified-Newton iteration. This option has no effect when the BFGS process is employed.

*TEMPERATURE

Nodal temperatures are read and used to generate thermal strains. These quantities are used also for the evaluation of creep strain and the integration of coupled creep-plasticity models such as Walker's model.

*THERMAL

Temperature dependent material properties are evaluated when this option is invoked, and the appropriate user subroutine is provided to the system prior to execution. This operation is not necessary for the conventional creep model since temperature dependence can easily be incorporated into the user subroutine CRPLAW.

*TRANSFORMATIONS

Coordinate transformations at nodal points are specified by this option in which the angle of rotation is to be prepared by the user so that the code can generate the necessary transformation matrices. The postprocessing file does not support coordinate transformations at this time.

*TYING

Multiple degree-of-freedom constraint equations are specified by the user through this option. This option is more flexible than the duplicated node option since constraints may be applied to individual degrees-of-freedom. Note that the constraint equations are generated only for the displacement degrees-of-freedom.

The following parameters are used to signal the MHOST program of the presence of specific user subroutines:

*UBOUN
*UCOEF
*UDERIV
*UFORCE
*UHOOK
*UPRESS
*UTEMP
*UTHERM

A brief description of each user subroutine is given below:

UBOUN specifies the prescribed displacement as a function of time and/or increment. This subroutine is called once for every increment, and the loop over the total number of constrained degrees-of-freedom must be included.

UHOOK specifies linear elastic material response varying with respect to node and temperature. This subroutine is called whenever the nodal stress is calculated.

UCOEF specifies anisotropic thermal expansion coefficients which may be given as functions of temperature. This subroutine is called whenever the nodal initial strain is calculated.

UPRESS is called at the beginning of every increment and specifies the distributed load varying with respect to time and/or increment.

UDERIV is an interface prepared for a user to add a special element in the form of the strain-displacement matrix. This subroutine is entered from the driver routine of the MHOST element library.

UTEMP specifies temperature dependent isotropic elasticity and thermal expansion. This subroutine is entered repeatedly at nodes from the linear elastic constitutive equation routine and the thermal strain routine.

UFORCE is executed at the beginning of every increment and specifies the prescribed nodal force as a function of time and/or increment. The loop over the total number of points at which force vectors are given must be coded into this subroutine.

UTHERM is called from the incremental analysis driver at the beginning of every increment to prescribe the nodal temperature field as a function of time and/or increment. The loop over the total number of nodes must be included.

As summarized above, the analysis capabilities included in the MHOST code cover most of the needs for inelastic calculation of turbine engine hot section components. Presently, the code consists of around 40,000 lines of FORTRAN statements including extensive, self-explanatory comment lines in each subroutine.

Table I summarizes the elements currently available in the MHOST code, Version 3.2, and parameters used to internally define the element characteristics. Further details are available in the MHOST Users' Manual.

3.4.3 Solution Algorithms

The line search algorithm has been implemented into the MHOST code. This option is available with any iterative solution scheme implemented in the code. As shown in the following example, it is not clear if the combined BFGS update - line search approach is the most efficient solution strategy in the present framework.

As shown in Table II, the line search technique improved the convergence characteristics dramatically for the cantilever beam problem (Figure 1). Improvement of the solution by the line search was no longer obvious when the scheme was applied to a prototype problem for three-dimensional shell structures as shown in Table III and Figure 2.

The inelastic response of the cantilever beam (Figure 1) is illustrated in Figure 3 and Table IV. The convergence behavior of the quasi-Newton, BFGS update was found to be superior to the Newton-Raphson type process, in which the tangent stiffness matrix was reformulated and factorized at every step of the iteration. It is important to note that the algorithm implemented here is far more efficient than Newton-Raphson type processes.

Table II

Elastic Beam: Convergence with Respect to Iteration

	Relative Residual			
	Constant Metric		Variable Metric (BFGS)	
Iteration Count	Constant Update	Line Search	Constant Update	Line Search
0	1.0	1.0	1.0	1.0
1	0.97637	0.47754-6	0.98028	0.11215
2	0.50296	0.12064-6	0.40637	0.22835-1
3	0.25836	0.98808-8	0.30279-2	0.13770-2
4	0.13250	0.30286-8	0.35640-4	0.27029-3
5	0.06790	0.35292-9	0.20975-7	0.16302-4

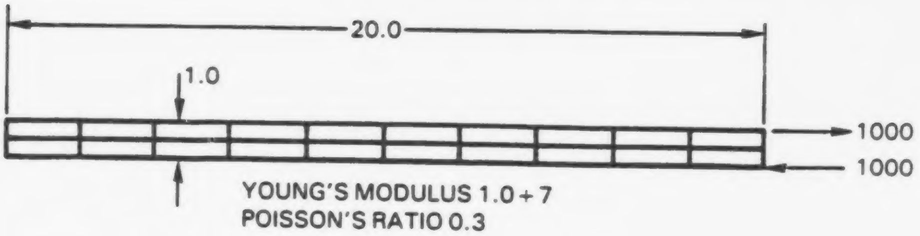

20.0
1.0
1000
1000
YOUNG'S MODULUS 1.0+7
POISSON'S RATIO 0.3

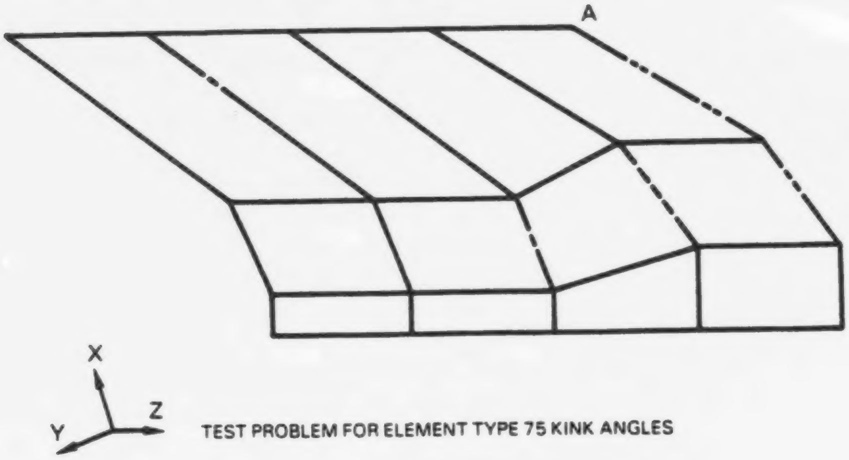
Figure 1 A Beam Problem - Linear Plastic Analysis

Table III

A Three-Dimensional Shell Problem

Convergence with Respect to Iteration

	Relative Residual				
	Constant Metric			Variable Metric	
Iteration Count	Constant Update	Line Search	Conjugate Gradient	BFGS	Secant Newton
0	0.51222 98.868	0.51222 98.868	0.51222 98.868	0.51222 98.868	0.51222 98.868
1	0.29682 60.786	0.17956 38.035	0.19521 41.186	0.28914 60.811	0.28322 56.219
2	0.19051 39.838	0.92278-1 19.521	0.13825 29.249	0.10905 23.421	0.72094-1 15.514
3	0.13140 27.729	0.56205-1 11.990	0.56362-1 12.150	0.45218-1 9.7468	0.31623-1 6.8351
4	0.93775-1 19.892	0.19583-1 4.1953	0.30214-1 6.4940	0.20974-1 4.5096	0.19135-1 4.1212
5	0.67875-1 14.445	0.15912-1 3.4039	0.17466-1 3.7416	0.13668-1 2.9369	0.16991-1 3.6519



TEST PROBLEM FOR ELEMENT TYPE 75 KINK ANGLES

Figure 2 A Three-Dimensional Shell Problem

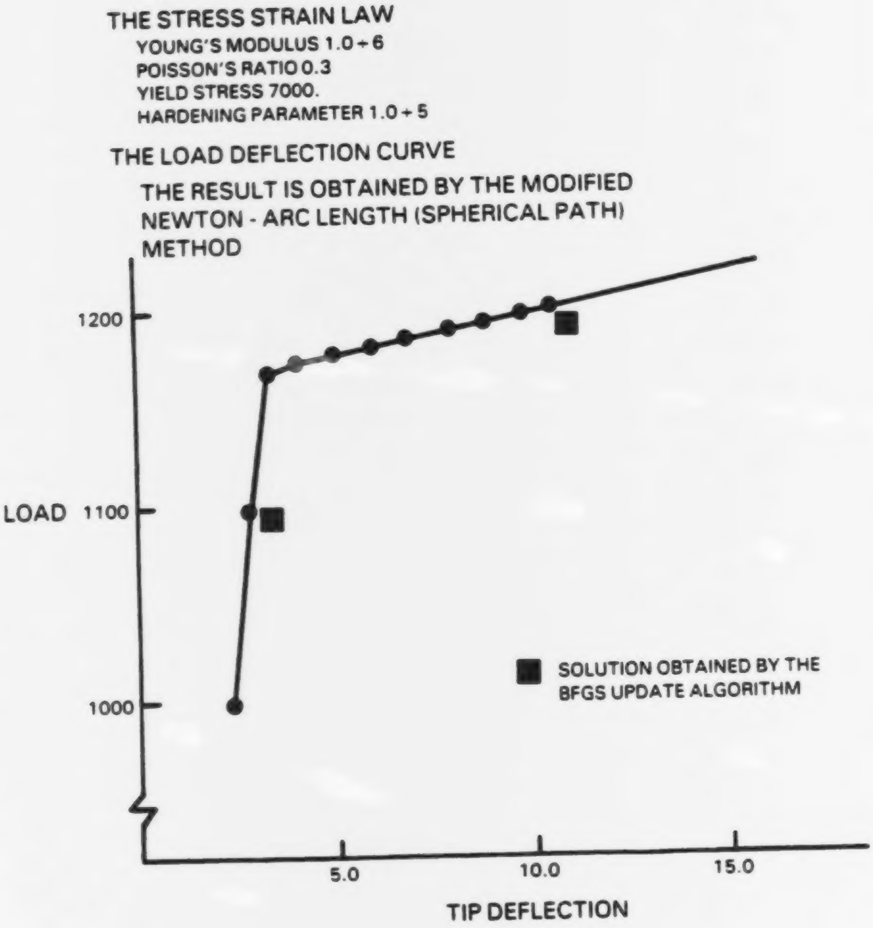


Figure 3 A Beam Problem - Elastic Plastic Analysis

Table IV

Solution of the Elastic Plastic Beam Problem

Method	Load Level	Number of Iterations	Normalized Tip Deflection
Newton Raphson, Constant Update	1.0	5	0.9917
	1.1	2	1.0997
	1.2	10	Fail to converge
Newton Raphson, Line Search	1.0	1	1.0000
	1.1	1	1.1000
	1.2	3	2.1937
	1.3	10	Fail to converge
Modified Newton Line Search	1.0	1	1.0000
	1.1	1	1.1000
	1.2	9	4.1340
	1.3	3	15.0842
	1.4	5	26.0958
	1.5	5	37.1663
Conjugate Gradient	1.0	1	1.0000
	1.1	1	1.1011
	1.2	10	Fail to converge
Quasi-Newton/BFGS Update, Constant Update	1.0	2	1.0023
	1.1	1	1.0985
	1.2	7	4.4550
	1.3	5	14.6930
	1.4	9	24.1375
	1.5	5	36.4625
Quasi-Newton/BFGS Update, Line Search	1.0	1	0.9997
	1.1	1	1.1016
	1.2	3	3.5301
	1.3	10	Fail to converge
Secant Newton/Davidon Update, Constant Update	1.0	2	1.0002
	1.1	3	1.1000
	1.2	6	4.4108
	1.3	10	18.5279
	1.4	9	24.7733
	1.5	7	34.7596
Secant Newton/Davidon Update, Line Search	1.0	1	1.0125
	1.1	3	1.1005
	1.2	7	5.8146
	1.3	3	16.7263
	1.4	10	Fail to converge

Note: Parameters are: Maximum Number of Iterations 10, Relative Residual Error Tolerance 0.1, and Relative Displacement Error Tolerance 0.05.

The line search algorithm was then improved to reduce the number of residual load evaluations in the iterative process. In addition, the accuracy of the search distance parameter was improved significantly. The numerical results obtained by the new version of the code are compared with corresponding values from the previous scheme in Table V for the 20-element plane stress model of a cantilever beam.

Table V

Elastic Beam: Convergence of Modified Line Search, Conjugate Gradient and Secant Newton Procedures

Iteration Count	Line Search (Old)	Line Search (New)	Conjugate Gradient	Secant Newton
0	1.0	1.0	1.0	1.0
1	0.47754-6	0.14709-7	0.14709-7	0.98772
2	0.12064-6	0.51162-8	0.51481-8	0.16435-1
3	0.98808-8	0.24806-8	0.25119-8	0.12846-3
4	0.30286-8	0.12944-8	0.13530-8	0.38142-10
5	0.35292-9	0.67459-9	0.12350-9	0.23028-10

The preconditioned conjugate gradient algorithm has also been included in the MHOST code. The performance of this procedure was compared against the line search algorithm, as shown in the third column of Table V. Convergence was extremely rapid with the residual monotonically decreasing. This procedure did not, however, offer a particularly attractive alternative for solving inelastic problems.

The secant-Newton method of the form derived from the Davidon rank-one quasi-Newton update has also been implemented into the MHOST code. This option is particularly attractive when compared with the quasi-Newton method since storage of update vectors is not required. The performance of this approach is included in Table I. The secant-Newton procedure converged faster than the BFGS scheme for this application.

It should be noted that utilization of variable metric iterations in the linear equation solution for finite element analysis has not yet appeared in the literature.

3.4.4 Frontal Solution Subsystem

Implementation of the frontal solution subsystem required a substantial coding effort that included a considerable amount of work associated with the reorganization of MHOST data structure. A core allocation routine was coded in conjunction with a driver routine to control the quasi-static analysis by the frontal solution subsystem. The previously available band matrix solution has been left untouched and existing data decks can be used without any modification.

The particular version of the frontal solver included in the MHOST code was designed for nonsymmetric indefinite systems of equations and utilizes diagonal pivoting within the front matrix. To avoid excessive read/write operations on a scratch file, a storage scheme was designed which utilizes the unused portion of work-space at the end of core-allocation as primary data storage. This space is referred to as the virtual disk file. Then the scratch file is assigned to secondary data storage, and read/write operations are carried out in a sequential manner. At the end of solution operations, the contents of the virtual disk are dumped to the scratch file, and this work space is released for other operations. This storage scheme is particularly efficient on machines without virtual memory but with high-speed secondary storage devices, such as the solid state device for CRAY computers.

The frontal solution subsystem currently supports the following algorithmic options: quasi-static analysis, line search, conjugate gradient, tying, and duplicate nodes.

A number of validation cases have been successfully executed on the PRIME 9950 at MARC under the Primos 19.4 operating system, and the results are summarized in Table VI. It is noted that the code was compiled using the FORTRAN-77 compiler prior to the testing, and it has also been compiled and tested with a FORTRAN-66 compiler.

In Table VI, the memory requirement entries exclude the space used as virtual disk space. In the validation cases, the beam problem and the prototype vane example were suitable for band matrix solution since they consisted of regularly connected elements. Hence, the frontal solution shows a slight increase in computational effort, but the memory was less than the band matrix solution. The advantage of the frontal solution became significant when complicated meshes were processed, particularly for cases with tying constraints which increased the computational effort significantly for the band matrix solver.

The program architecture related to the frontal solution subsystem is now summarized. The numerical treatment of duplicate nodes, tyings and transformations was significantly different from corresponding operations for these effects implemented in the band matrix subsystem.

Table VI

Performance Tests for Frontal Solution Subsystem

	Solver*	Memory Requirement (Words)	Central Processing Unit Time (Seconds) Data Input	Solution
2-D Elements Model For A Beam	B	10195	0.952	0.824
	F	9541	0.942	0.831
Prototype Vane Model	B	46189	1.100	5.300
	F	37559	1.121	5.670
Plate With A Hole	B	12277	1.000	1.300
	F	9617	1.024	1.103
L-Shape Domain (Continuous Stress)	B	27841	1.645	3.237
	F	18043	1.712	2.746
L-Shape Domain (With Tying Option)	B	34459 (17404)	1.782	4.747
	F	18695 (1626)	1.839	3.568

* B: Band Matrix
F: Frontal Solution

The penalty function method was used to impose algebraic constraints of the duplicate node and tying types. Internally, an element consisting of two nodes was generated for each constraint data line in the connectivity data array. The stiffness coefficient was taken as 10^5 times the value of the elastic modulus associated with the master node. Forward reduction was performed first for every regular element, and then these constraint elements were processed in a single stream of operations.

The coordinate transformations were carried out on an element-by-element basis. When the element equations are assembled, a test is performed to determine if any one of the nodal points is subjected to the transformation and then the appropriate transformation operation is performed.

For validation of these capabilities, a number of simple numerical tests were performed at MARC and the results were satisfactory, reproducing the same numbers as the band matrix option up to the fifth significant digit.

A MARC generated model of a three-dimensional burner blister specimen was also used to test the performance of the frontal solution subsystem. As shown in Figure 4, the model consists of 316 eight-noded hexahedral elements, 603 nodes and 123 nodal coordinate transformations. This example was also used to test the postprocessing file interface. The element renumbering to reduce the frontal matrix size was performed using an intuitive element renumbering scheme which involved geometrically sweeping the element identification from the center of the model to the outer circle. The statistics were:

	Band Solution	Frontal Solution
Core storage (32 bit-words)	569,853	295,403
CPU time (seconds) per iteration	157.8	201.5
Tip deflection		
(0 iteration)	0.50719-3	
(4 iterations)	0.54622-3	

The profile of the computed stress field has been successfully produced on the graphic postprocessing subsystem as shown in Figure 5.

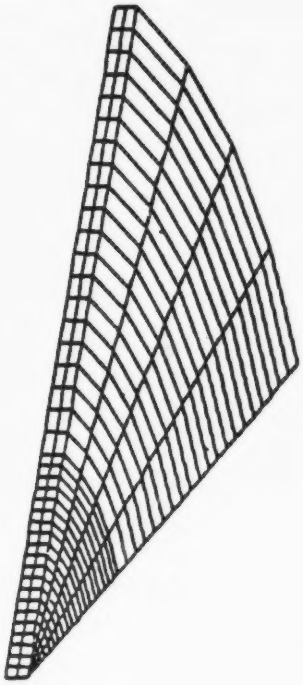


Figure 4 MARC Blister Specimen Model

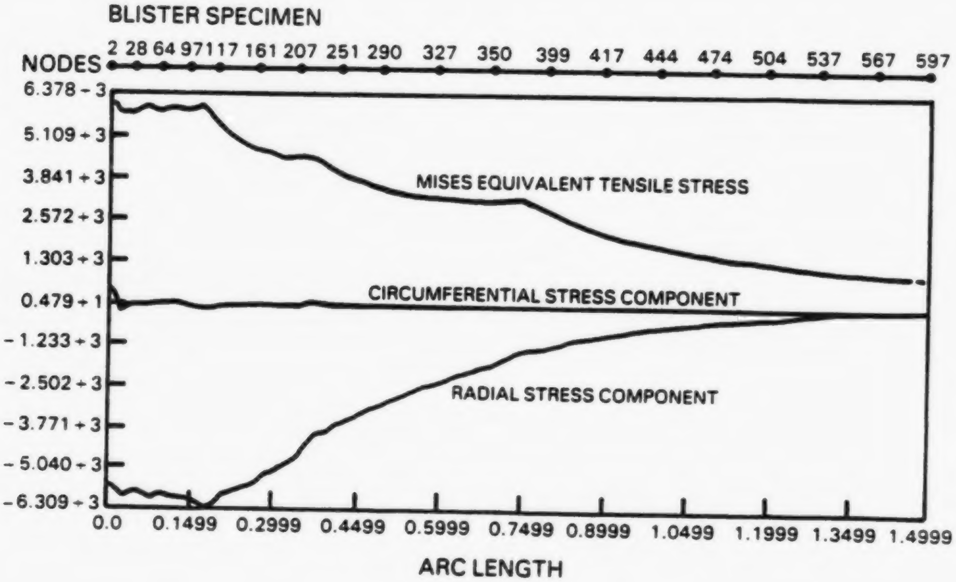


Figure 5 Mises Stress for Blister Specimen

3.4.5 Anisotropic Material Property Reader

At the request of the Contract Monitor at NASA-LeRC, a user-friendly format to deal with anisotropic material properties and composite laminate plates and shells has been added to the MHOST code.

3.4.5.1 Composite Laminate Option

The composite laminate option has been completed, including a simple validation run. The material property data for the laminates are read directly into the elastic modulus array for shell elements in the format discussed in the paper Munich, Chamis (1975). For validation purposes, an example included in the above reference was solved. A cantilever beam made of a composite laminate is modeled using shell element type 75 in conjunction with *COMPOSITE and *LAMINATE options.

The geometry and finite element model are illustrated in Figure 6 and the input data file is as follows:

```
VALIDATION CASE FOR COMPOSITE LAMINATE OPTION

C

C    EXAMPLE FOUND IN M.D.MINICH AND C.C.CHAMIS (1975) -

C    ANALYTICAL DISPLACEMENTS AND VIBRATIONS OF CANTILEVERED UNSYMMETRIC

C    FIBIRE COMPOSITE LAMINATES, NASA TECHNICAL MEMORANDUM NASA TMX-

C    71699

C
```

```
*ELEMENT 8
  75
*COMPOSITE
*NODES      15
*BOUNDARY CONDITIONS    50
*FORCE                  30
*END
*ITERATION
     5    0.05     0.00      0.01
*COORDINATES
     1    0.0     -0.5       0.0       0.1
     2    0.0      0.0       0.0       0.1
     3    0.0      0.5       0.0       0.1
     4    0.5     -0.5       0.0       0.1
     5    0.5      0.0       0.0       0.1
     6    0.5      0.5       0.0       0.1
     7    1.0     -0.5       0.0       0.1
     8    1.0      0.0       0.0       0.1
     9    1.0      0.5       0.0       0.1
    10    1.5     -0.5       0.0       0.1
    11    1.5      0.0       0.0       0.1
    12    1.5      0.5       0.0       0.1
    13    2.0     -0.5       0.0       0.1
    14    2.0      0.0       0.0       0.1
    15    2.0      0.5       0.0       0.1
```

```
*ELEMENTS 75
    1    1    4    5    2
    2    2    5    6    6
    3    4    7    8    5
    4    5    8    9    6
    5    7    10   11   8
    6    8    11   12   9
    7    10   13   14   11
    8    11   14   15   12
*PROPERTIES 75
    1     8    1.00000   0.00001   0.00001   0.00001
*LAMINATE
C
C     CASE VI  IN THE REFERENCE
C
     1  15
2315.E+3    24.E+3   0.E+3  2315.E+3   0.E+3   82.E+3   37.E+3   37.E+3
 -55.E+3     0.E+3   0.E+3    55.E+3   0.E+3    0.E+3    0.E+3    0.E+3
1929.E+0    20.E+0   0.E+3  1929.E+0   0.E+0   68.E+0   31.E+0   31.E+0
*BOUNDARYCONDITIONS
     1    1
     1    2
     1    3
     1    4
     1    5
```

```
        1   6
        2   1
        2   2
        2   3
        2   4
        2   5
        2   6
        3   1
        3   2
        3   3
        3   4
        3   5
        3   6
  *FORCE
     13    3    15.0
  *PRINT
     TOTAL
     STRESS
     STRAIN
  *END
  *STOP
```

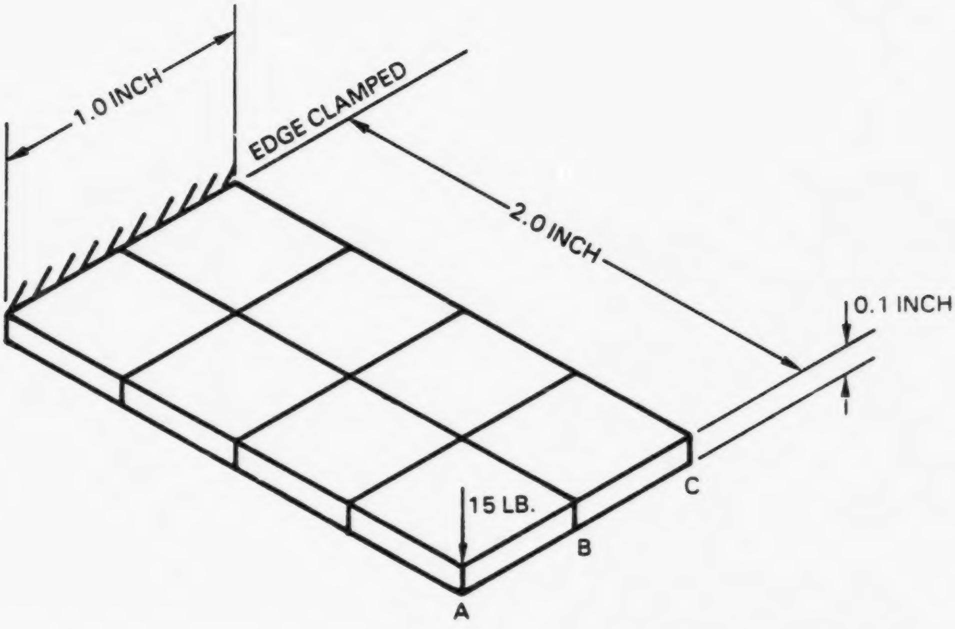


Figure 6 Composite Beam Model Geometry and Finite Element Mesh

The material is Thornel-75-S/epoxy with a fiber volume ratio of 0.6. For the details of ply orientation, refer to the comment lines of the input data deck. Each nodal point has the same set of material properties as assigned by the *LAMINATE data segment. After four iterations, a relative residual of 0.049835 is reached and the tip displacements are:

		0th Iteration	4th Iteration	Reference
At Point	A	0.0888	0.0929	0.0887
	B	0.0628	0.0658	0.0644
	C	0.0421	0.0444	0.0434

where Reference indicates the displacement results reported in Minich and Chamis (1975), who used the six-noded quadratic triangles in a 16-element 45-node mesh. For comparison purposes, an uncoupled model was constructed, resulting in deflection values of:

		2nd Iteration	Reference
At Point	A	0.0427	0.0405
	B	0.0211	0.0212
	C	0.0035	0.0036

3.4.5.2 Anisotropic Elastic Material Reader

With the user subroutine UHOOK residing in the MHOST code, the user can specify any set of anisotropic elastic properties. An improved user interface has been developed which reads the entries of material modulus directly instead of invoking UHOOK. The additional model data parameter *DMATRIX invokes the subroutine DMATIN which interprets the numerical data discussed below. This option is available for continuum elements as well as for shell elements where the *COMPOSITE and *LAMINATE options must also be invoked.

The data format is:

*DMATRIX	This data line invokes the direct material modulus data reader at nodes. (NELSTR + 1) numeric data lines follow.

The first data line includes two integers indicating the series of nodes at which the code will apply the material property data to follow:

Integer 1:	The first node in the series.
Integer 2:	The last node in the series.

If the second integer is zero or left blank, the following material property data are applied only at the node specified by the first integer entry.

Subsequent data lines consist of NELSTR real entries for each row of the D matrix at the nodes specified by the first data line.

3.4.6 Coordinate Transformations

The coordinate transformation process used for the selective integration scheme was modified to improve the performance of the linear Lagrangian elements used in MHOST. The polar decomposition formula for the two-dimensional Jacobian matrix was rewritten using the Cayley-Hamilton theorem.

The numerical performance of the element implemented in the current version of the MHOST code was compared with that of the hybrid stress element proposed by Pian, Sumihara (1984), in which the element bending modes were dealt with in the isoparametric coordinate system. The example used here, Figure 7, was the pathological one discussed in this paper. Note that a=1 means the angle of distortion is 45 degrees, the usual limit used in practical computations. For the range of distortion typically occurring in engineering computations, the preconditioning system did not perform as well as the rational hybrid stress element. However, the iterative algorithm generally outperformed the hybrid element as shown in Figure 7.

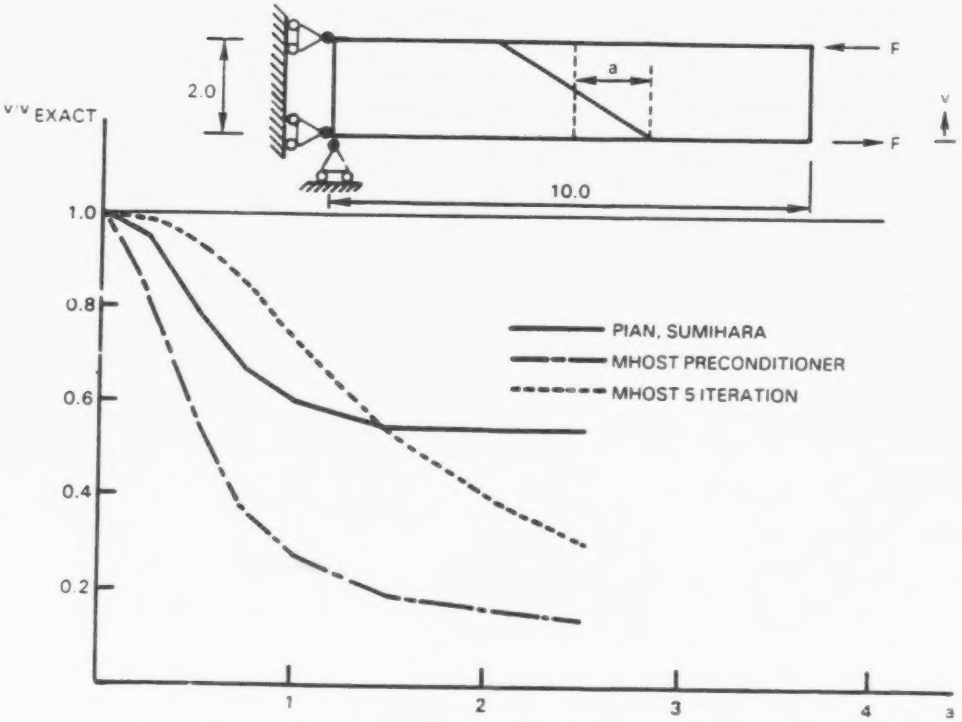


Figure 7 MHOST Selective Integration Versus Pian Rational Hybrid Stress

3.4.7 Subelement Development

Subelement Solution Procedure

In the subelement region, the mixed finite element equations are constructed and solved iteratively. The displacement preconditioning is carried out in terms of the hierarchical nodal displacements in order to generate the incremental displacements in the subelement regions. Care is exercised to ensure that the effects of thermal and creep strains are correctly incorporated into the subelement load vector.

Incremental strains are recovered at subelement nodes using a variational recovery process. Note that continuity of strain is no longer assumed over the global nodal points to which more than one subelement is connected.

The constitutive equation is also integrated at subelement nodes using the subelement nodal strains. The contribution of thermal and creep strains is evaluated by using the subelement nodal temperatures interpolated from the global nodal temperatures specified by the user. The total and incremental stresses are stored at the subelement nodal points.

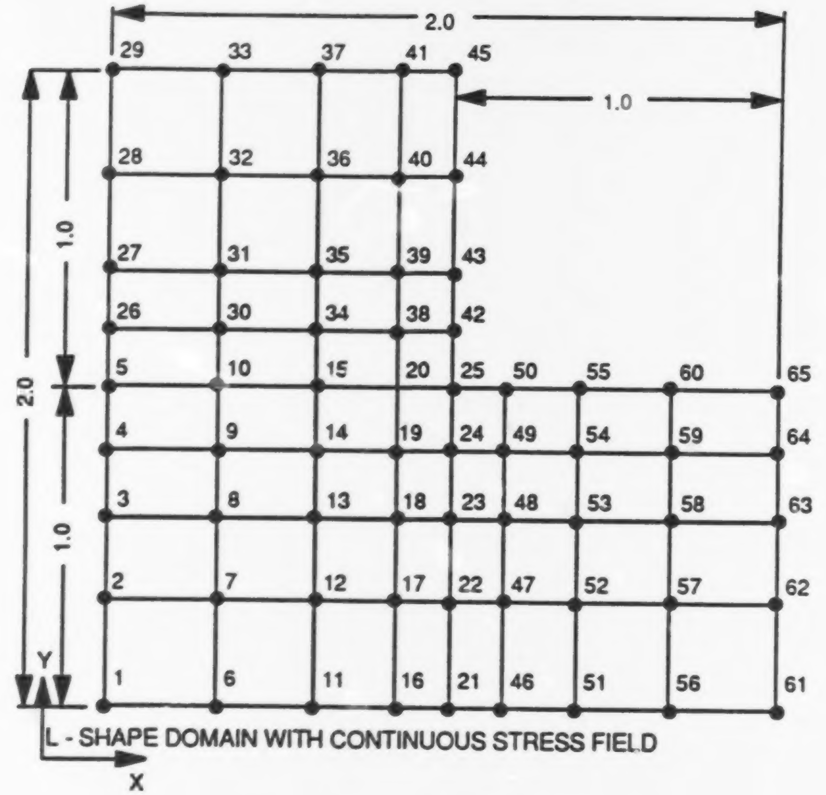
The subelement solution is coupled to the global finite element process through equilibrium iteration. The numerical integration procedure for the residual load vector plays an important role in controlling the overall behavior of the numerical solution.

Two options are available to the user to control this coupling. The weak coupling scheme uses Gauss quadrature together with a simplified bilinear representation of the stress field. This scheme satisfies all the patch test requirements but its ability to extract local stress concentrations is not satisfactory. The strong coupling scheme, which does not satisfy the patch test for irregular meshes at this time, employs a special trapezoidal integration. The algorithm integrates the residual weighted by the area, which is conveniently available as the local nodal strain projection operator. Experience with the strong coupling scheme has led to modifications involving changes in weight factors. As the numerical example in the next section indicates, this modified strong coupling scheme detects stress concentrations effectively. However, the modified strong coupling scheme still slightly overestimates the residual when the contribution of the shear deformations of elements is significant. Further improvements are necessary and will be the subject of future investigations.

The first validation problem consists of a corner singularity in a plane stress setting. Two global finite element meshes were generated. The coarse grid refers to the finite element mesh used in previous validation runs including 48 bilinear mixed Type 3 elements (Figure 8). The fine mesh was generated by subdividing all the elements in the coarse grid into 2 by 2 bilinear elements. The subelement mesh refers to the coarse mesh with each of the three elements around the singular point represented by a 2 by 2 subelement grid.

At the singular point (re-entrant corner in the L-shape domain), the tying option is used to disconnect the strain and stress fields and, hence, the stress field can be approximated in an accurate fashion.

The convergence characteristics are summarized in Table VII in terms of the relative residual. It is interesting to note that the BFGS update scheme diverges when applied to this problem. The solution at the singular point is summarized in Table VIII. A slight improvement of the nodal stress is observed in the subelement solution.


2.0
1.0
1.0
1.0
2.0
Y
X
29
33
37
41
45
28
32
36
40
44
27
31
35
39
43
26
30
34
38
42
5
10
15
20
25
50
55
60
65
4
9
14
19
24
49
54
59
64
3
8
13
18
23
48
53
58
63
2
7
12
17
22
47
52
57
62
1
6
11
16
21
46
51
56
61

L - SHAPE DOMAIN WITH CONTINUOUS STRESS FIELD

E = 10^7; $\nu = 0.3$
LINEAR ELASTICITY ASSUMED

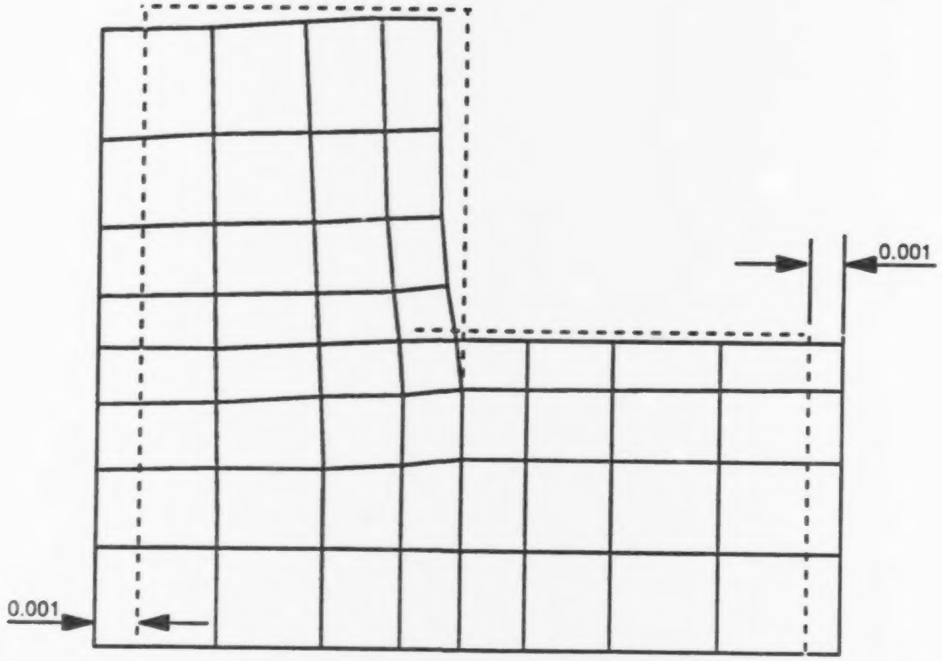


Figure 8 Problem Statement for Plane Stress Deformation of a Domain with a Singularity

Table VII

Convergence of the Global Iteration for the Elastic Analysis of the L-Shape Domain (Prescribed Relative Residual Tolerance 0.01)

Iteration Count	Coarse Mesh	Fine Mesh	Subelement Mesh
(I) Constant Metric Iteration			
0	0.87591-1	0.94754-1	0.63856-1
1	0.48559-1	0.48205-1	0.41864-1
2	0.38770-1	0.39204-1	0.27499-1
3	0.33447-1	0.34712-1	0.18950-1
4	0.30079-1	0.31803-1	0.13658-1
5	0.27713-1	0.29526-1	0.10200-1
6	0.25930-1	0.27699-1	0.81305-2
7	0.24518-1	0.26194-1	
8	0.23360-1	0.24518-1	
9	0.22380-1	0.23839-1	
10	0.21531-1	0.22893-1	
(II) Secant Newton (Davidon Rank One) Iteration			
0	0.87591-1		0.63856-1
1	0.48559-1		0.41865-1
2	0.28219-1		0.15284-1
3	0.26842-1		0.11587-1
4	0.27726-1		0.61043-2
5	0.24590-1		
6	0.19135-1		
7	0.18115-1		
8	0.17086-1		
9	0.14330-1		
10	0.10645-1		

Table VIII

Stress and Displacement Solution: L-Shape Domain

(I) Displacement at the Singular Point

	X-Displacement	Y-Displacement
Coarse Mesh	-0.26425-3	-0.14922-3
Fine Mesh	-0.25998-3	-0.13495-3
Subelement Mesh	-0.27157-3	-0.14972-3

(II) Mises Equivalent Stress at the Singular Point. Note that duplicate nodes at the singular point result in different stress values at the same point.

		( ) refined mesh solution
	(17484.)	
Global	12539.	
Global/Local	11440.	
Subelement	12589.	
	B	
	A	C
	(11638.)	(25634.)
Global	9296.	19782.
Global/Local	9316.	19148.
Subelement	9621.	20463.

Table IX summarizes the results obtained by the modified integration scheme discussed above for both the global and subelement schemes. In the table, points A, B and C indicate the duplicate nodes at singular points in the bottom left, top left and bottom right elements, respectively. As indicated clearly, the stress values obtained by the subelement schemes are consistently higher than the finer mesh solution. This result qualitatively indicates that the modified integration scheme is now capable of detecting the stress field effectively and also properly transmits the subelement information to the global finite element solution. The quadratic subelement results show superior performance when compared to the linear subelement results.

The above observations are preliminary and further quantitative numerical investigations need to be conducted. Possible code modifications to parameterize uniform subelement mesh generation will be considered to boost the performance of this procedure.

The validation of the subelement code for three-dimensional analysis was carried out using a three-dimensional block under uniform mechanical and thermal loading as shown in Figure 9. The code produced the exact theoretical results for displacement, strain and stress.

Table IX

Stresses at the Re-Entrant Corner

	Mises Equivalent Stress Value		
	Point A	Point B	Point C
Coarse Mesh	9.296+3	12.539+3	19.782+3
Fine Mesh	11.638+3	17.484+3	25.634+3
Coarse Mesh With Linear Subelement			
Global Node	12.598+3	14.828+3	24.979+3
Subelement Node	14.085+3	18.468+3	30.901+3
Coarse Mesh With Quadratic Subelement			
Global Node	13.846+3	15.707+3	27.829+3
Subelement Node	14.949+3	22.391+3	35.750+3

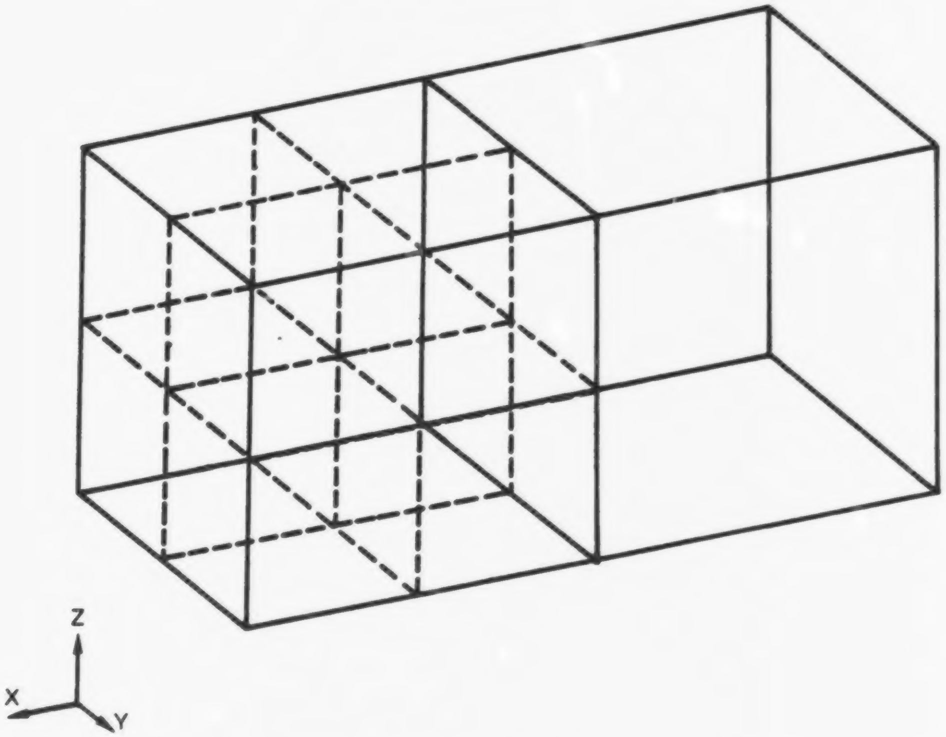


Figure 9 Three-Dimensional Subelement Validation

Quadratic Subelement Technology

In this section, the validation of the quadratic subelements is discussed. To integrate the stiffness equations for quadratic Lagrangian elements, full 3 by 3 Gaussian quadrature is implemented, whereas reduced 2 by 2 quadrature is used to recover the nodal strain. The validation cases reported here are limited to plane stress problems. In the range of numerical experiments discussed here, the above integration schemes are found to produce satisfactory numerical results. Further numerical study is necessary to construct an optimal integration procedure for quadratic elements.

A series of two-dimensional numerical test cases was carried out for linear elastic and elastic-plastic problems. The results of a linear elastic beam analysis are summarized in Table X. The numerical model was the 20 plane stress element representation of the structure of which the two global elements on the fixed end were subdivided into both linear and quadratic subelements as shown in Figure 10. Note that exact values were reproduced at the nodes, although continuity of the displacement on the interelement boundary is not explicitly enforced except at the nodes.

Table X

Beam Problem: Subelement Validation

		Finite Element Solution		
X-Coordinate	Exact Deflection	Global	Linear Subelement	Quadratic Subelement
0.0	0.0	0.0	0.0	0.0
0.5	0.0015	(0.0060)	(0.0030)	0.0015
1.0	0.0060	(0.0120)	0.0060	0.0060
1.5	0.0135	(0.0180)	(0.0150)	0.0135
2.0	0.0240	0.0240	0.0240	0.0240

Note: Values indicated by ( ) are based on the nodal value calculated by the finite element interpolation functions.

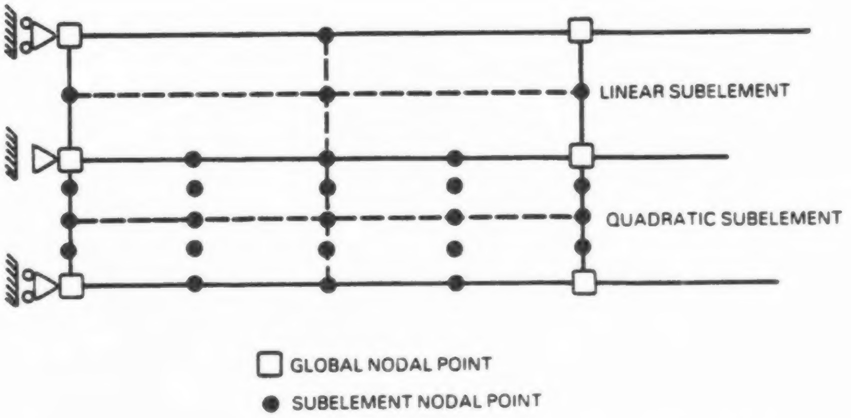
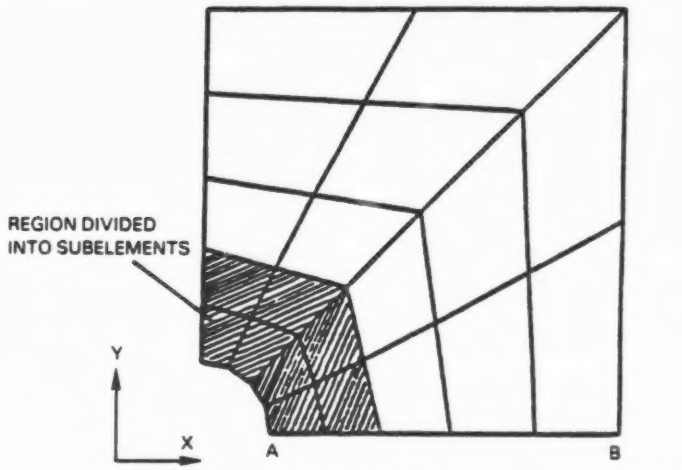


Figure 10 Subelement Refinement for the Beam Problem

The elastic deformation of a plate with a hole subjected to a uniform tensile load was studied using various finite element models. The basic mesh is shown in Figure 11 with the subelement division indicated by symbols. The stress distribution without any subelement refinement along the edge is shown in Figure 12 and the Mises equivalent strain contour plotted in Figure 13. Figures 14 and 15 represent the same information obtained from the uniformly linearly subdivided subelement mesh. The numerical values obtained from these analyses are summarized in Table XI.


REGION DIVIDED INTO SUBELEMENTS
Y
X
A
B

HOLE IN PLATE UNDER IN PLANE LOAD — MHOST SETUP

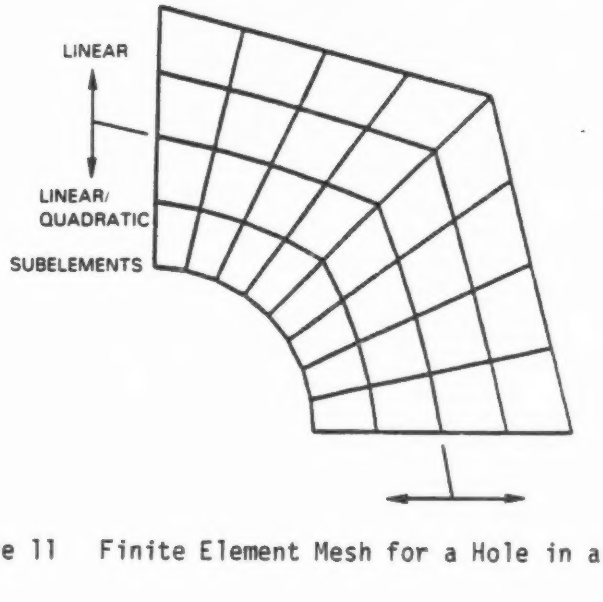

LINEAR
LINEAR/ QUADRATIC
SUBELEMENTS

Figure 11 Finite Element Mesh for a Hole in a Plate

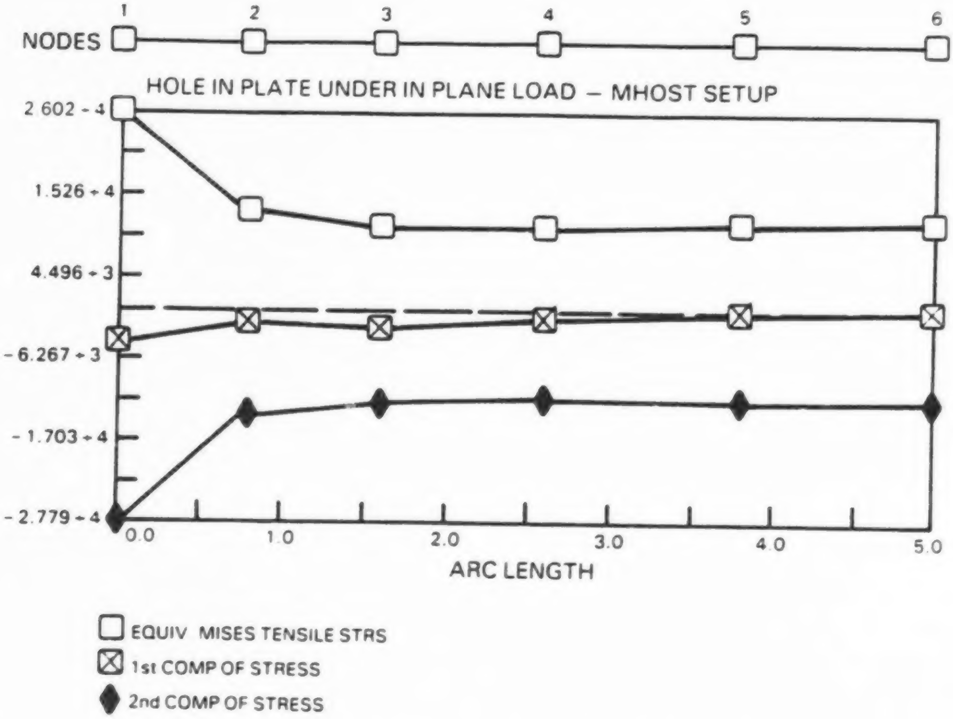


Figure 12 Stress Distribution Along the Edge A - B Global Mixed Solution with Coarse Mesh

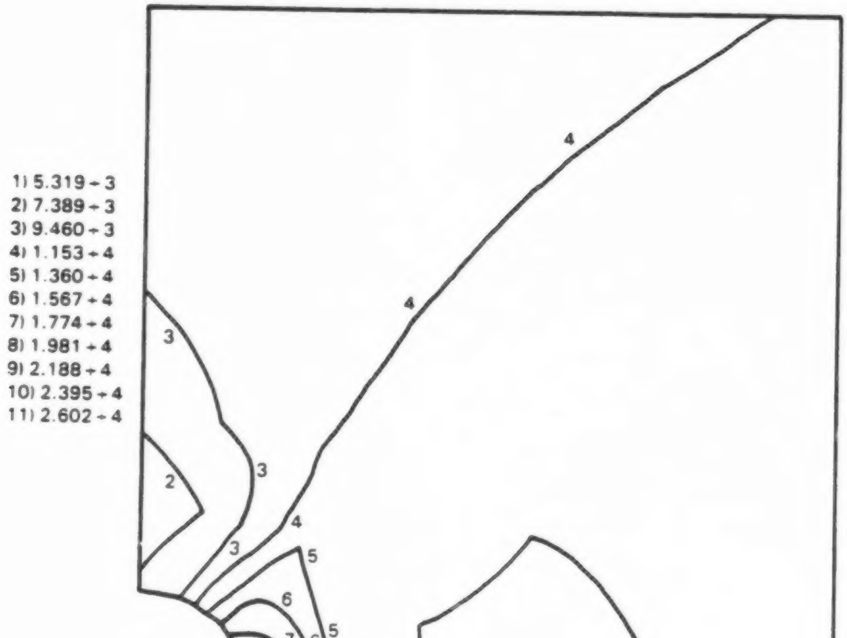


Figure 13 Mises Equivalent Stress Global Mixed Solution with Coarse Mesh

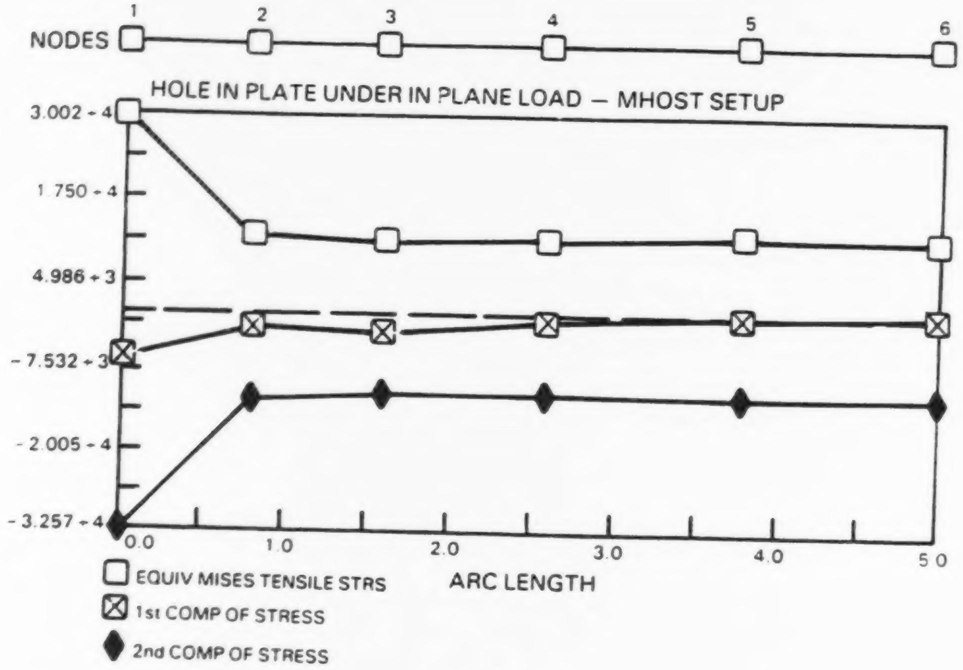


Figure 14 Stress Distribution Along the Edge A - B: Coarse Mesh with Linear-Quadratic Subelement Division

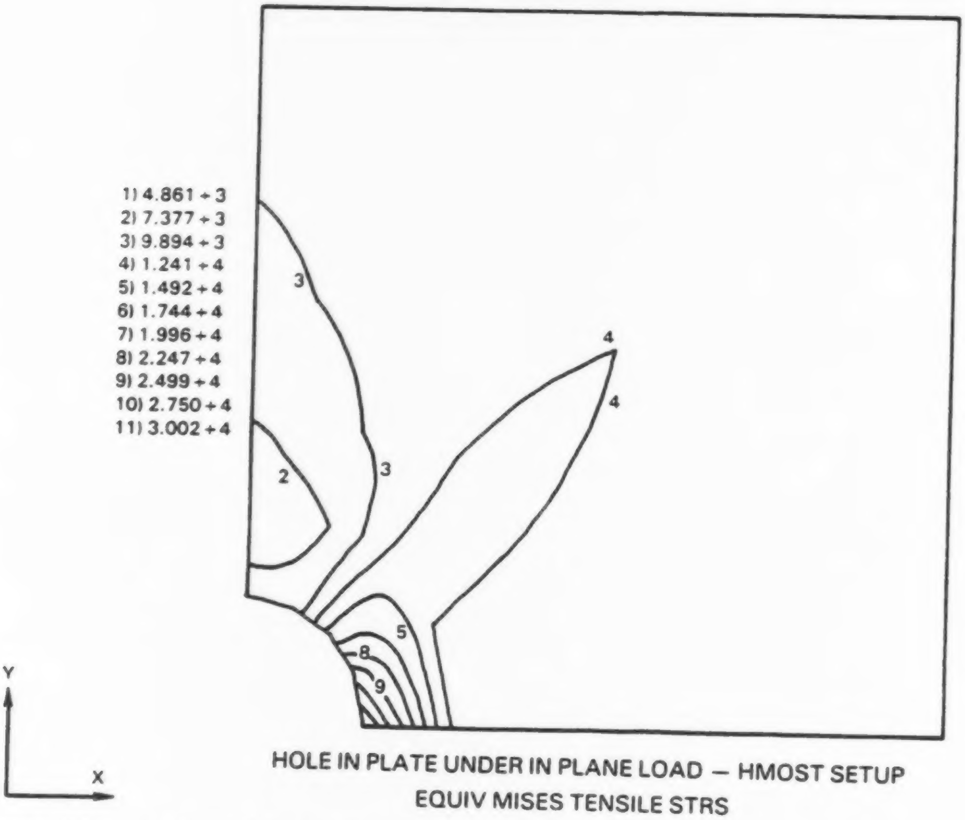


Figure 15 Mises Equivalent Stress: Coarse Mesh with Linear-Quadratic Subelement Division

Table XI

Elastic Stress Analysis of a Plate and a Hole:
Stress and Strain at the Edge (Point A on Figure 10)

	Equivalent Mises Stress	Horizontal Displacement
Global Mixed Solution		
Coarse Mesh	2.6026+4	0.30068-3
Fine Mesh	2.9382+4	0.34386-3
Linear-Linear Subelement		
Global Node	3.0054+4	0.34912-3
Subelement Node	3.0059+4	0.34912-3
Quadratic-Linear Subelement		
Global Node	3.0026+4	0.35232-3
Subelement Node	3.0070+4	0.35232-3

Subelements for Embedded Holes

A generalized version of the hole subelement has been fully implemented, and validation runs have been made. It is now possible to specify the number of subelement divisions in the radial direction (denoted by NUMRAD) and on the element edges (NUMEDG). Figure 16 shows the configuration of a subelement mesh for NUMRAD = 2 and NUMEDG = 2. The diameter of the hole and the subelement type (either linear or quadratic) are the user-definable parameters for each hole subelement.

The first validation case involved an analysis of stress concentration around a hole in a square plate. A uniform axial load was applied on the right hand edge, and the horizontal displacement was constrained on the left hand edge. The vertical displacement was constrained at the left bottom corner. A uniform nine-element mesh was prepared as shown in Figure 17 in which the element at the center of the plate was subdivided into the subelement grid as shown in Figure 16. The result of this subelement solution was compared with the global finite element solution obtained from the reference mesh, as shown in Figure 18.

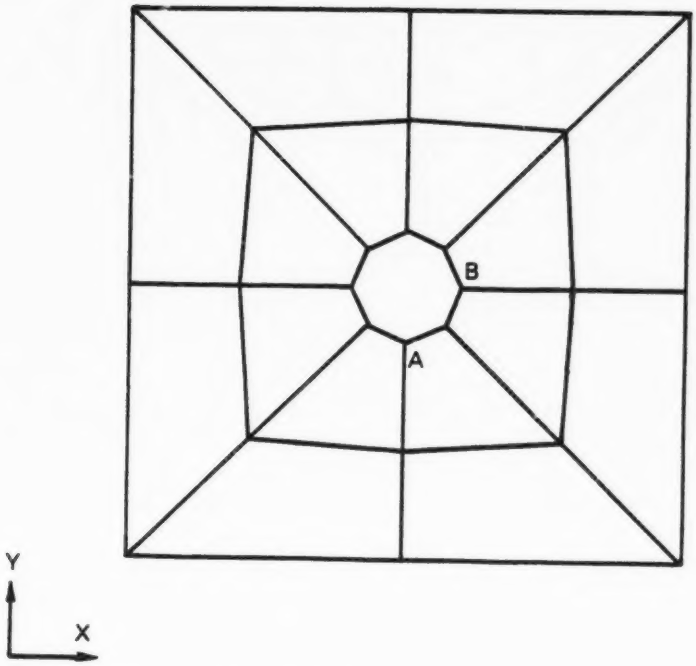


Figure 16 Subelement Mesh for a Hole

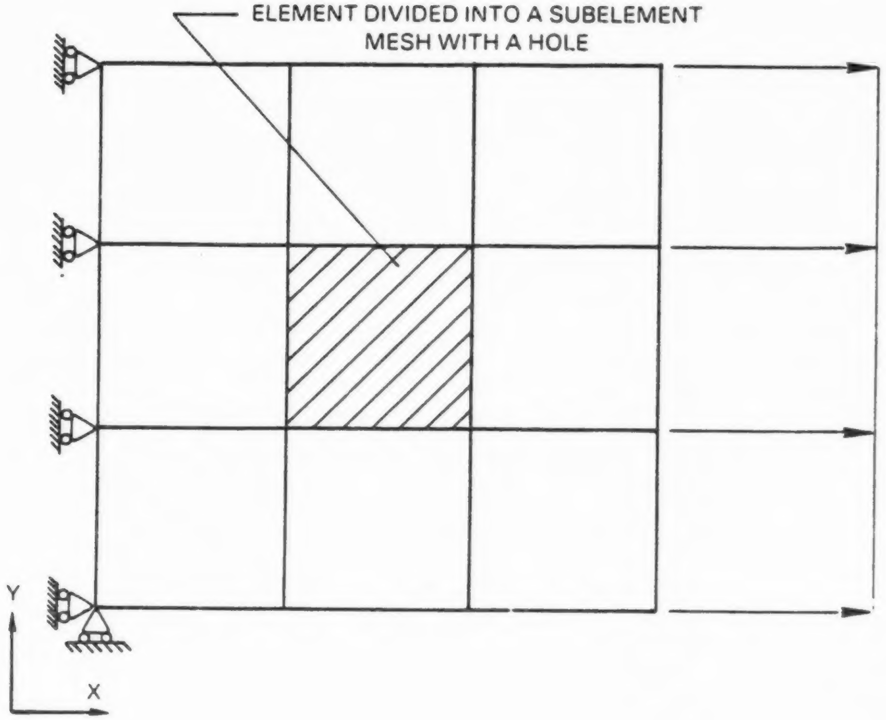

ELEMENT DIVIDED INTO A SUBELEMENT MESH WITH A HOLE
Y
X

Figure 17 Global Finite Element Mesh

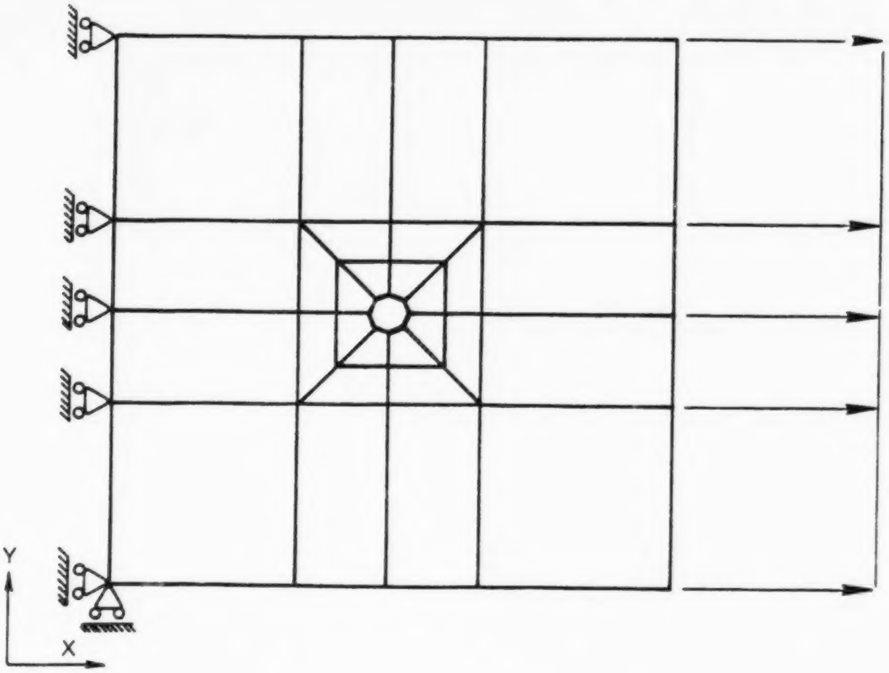


Figure 18 Standard Finite Element Model with a Hole

The initial solution of the model with an embedded hole was the uniform uniaxial state of stress with the displacement linearly increasing in the horizontal direction. In the residual force recovery phase of the mixed iterative operation, the subelements representing the hole produced out-of-balance forces at internal nodes. These forces represent the reduction in stiffness caused by the presence of the hole. The resultant forces were used in the equilibrium iteration to update the global nodal displacement.

Stresses at points A and B of Figure 16 are presented in Table XII. The values are normalized by the uniform stress in a plate without a hole. As the tabulated values show, the subelement solution produced results consistent with corresponding results from the standard finite element solution.

Table XII

Nodal Stress at the Edge of the Circular Hole

	Global Solution	Subelement Solution	
		Linear	Quadratic
Point A			
σ_x	2.2615	2.3198	2.7087
σ_y	0.5916	0.5977	0.3929
τ_{xy}	0.0002	0.0000	0.0003
Point B			
σ_x	0.1752	0.4339	-0.2702
σ_y	-0.0813	-0.2995	-0.5958
τ_{xy}	0.0000	0.0000	0.0000

Anisotropic Plasticity

The generalization of the Mises yield criterion by Hill (1950) is implemented in the framework of the mixed, iterative solution approach.

The anisotropic Mises equivalent stress with respect to the rectangular coordinates parallel to the material axes is defined by

$$a_1(\sigma_{22} - \sigma_{33})^2 + a_2(\sigma_{33} - \sigma_{11})^2 + a_3(\sigma_{11} - \sigma_{22})^2$$

$$+ 3a_4\sigma_{23}^{\;2} + 3a_5\sigma_{31}^{\;2} + 3a_6\sigma_{12}^{\;2} = 2\tilde{\sigma}^2$$

For plane stress problems, the formula is reduced to

$$a_1\sigma_{22}^{\;2} + a_2\sigma_{11}^{\;2} + a_3(\sigma_{11} - \sigma_{22})^2 + 3a_6\sigma_{12}^{\;2} = 2\tilde{\sigma}^2 ,$$

where a_k ($k = 1, 2, \ldots, 6$) are defined as follows in terms of two vectors $\mathbf{d}$ and $\mathbf{h}$ which indicate the change in shape of the yield surface due to the anisotropic response of the material:

$$a_1 = \frac{1}{d_2^{\;2}} + \frac{1}{d_3^{\;2}} - \frac{1}{d_1^{\;2}}$$

$$a_2 = \frac{1}{d_3^{\,2}} + \frac{1}{d_1^{\,2}} - \frac{1}{d_2^{\,2}}$$

$$a_3 = \frac{1}{d_1^{\,2}} + \frac{1}{d_2^{\,2}} - \frac{1}{d_3^{\,2}}$$

and

$$a_4 = \frac{2}{h_3^{\,2}} \quad a_5 = \frac{2}{h_2^{\,2}} \quad a_6 = \frac{2}{h_1^{\,2}}$$

Note that isotropic Mises plasticity is recovered by setting each component of **d** = 1 and each component of **h** = 1.

The anisotropic formulation just described is suitable, for example, for modelling the behavior of sheet metal processed by rolling. This manufacturing process is likely to induce orthotropic anisotropy for the directions perpendicular to the roll. Further details on the physical assumptions involved in the generalized anisotropic plasticity model are presented in Hill (1950). Application of such a material model in finite element computations can be found in several commercially available general purpose finite element codes such as MARC.

The cantilever beam problem, as defined in Figures 1 and 3 and loaded to undergo elastic-plastic deformation, is used as the validation case for this capability. An incremental load equal to 10% of the initial elastic load (i.e. the same incremental setting as used in the example summarized in Table IV) is applied for five consecutive increments and the secant-Newton/Davidon rank-one quasi-Newton update scheme is used in each increment. The material axes are assumed oriented parallel with the global coordinate directions.

Under pure bending moment loading, the beam undergoes only elastic deformation up to load level 1.1. For the isotropic plasticity assumption, plastic behavior begins between load levels 1.1 and 1.2. Under these conditions, the x-direction stress component (σ_x) predominates at the locations on both the top and bottom surfaces of the beam, with the y-direction stress component (σ_y) at these locations being smaller by one or two orders of magnitude. No shear stress occurs in this deformation process. To validate the implementation of the anisotropic plasticity option into the MHOST code, four sets of results have been generated. As a reference solution, the stress history for a standard isotropic plasticity model is calculated in a standard manner, the results of which are shown in Column 1 of Table XIII. In this table, the x-stress component (σ_x), as well as the corresponding equivalent Mises stress ($\overline{\sigma}$) values are given at load levels up through 1.5. The anisotropic plasticity option in the MHOST code is then exercised directly by making each component of both **d** and **h** take the value 1.0. As indicated by the results in Column 2 to Table XIII, isotropic plasticity is fully recovered using the anisotropic plasticity option with these special **d** and **h** vectors.

Material anisotropy is fully introduced in the remaining two sets of results. For Column 3 of Table XIII, the effective yield surface is extended by 50% in the global x-direction. This is accomplished by setting $d_1 = 1.5$, so that the equivalent Mises stress values become much lower due to the reduced contribution of the predominant x-stress component (σ_x). From Column 3 of Table XIII, it can be seen that the equivalent Mises stress value, even at the highest load level shown, i.e. 1.5, still has not reached the yield level. On the other hand, the results are far less sensitive to the effective yield surface being extended by 50% in the global y-direction. This is accomplished by setting $d_2 = 1.5$ for the in-plane direction perpendicular to the beam. The extension by 50% in this direction alters the equivalent Mises stress values only very slightly as the load is increased. As can be seen from Column 4 of Table XIII, the solution starts to deviate from the isotropic response at load level 1.4 but only ever so slightly in the fifth significant figure.

Table XIII

Isotropic and Anisotropic Plastic Response of a Cantilever Beam

Load Level		Isotropic Plasticity	$\mathbf{d} = \mathbf{h} = 1$	Anisotropic Plasticity $d_1 = 1.5^{*1}$	$d_2 = 1.5^{*1}$
1.0	σ_x	5998.8	5998.8	5998.8	5998.8
	$\bar{\sigma}$	6002.9	6002.9	4001.9	6002.9
1.1	σ_x	6613.8	6613.8	6613.8	6613.8
	$\bar{\sigma}$	6568.2	6568.2	4379.3	6568.2
1.2	σ_x	7086.1	7086.1	7221.6	7086.1
	$\bar{\sigma}$	7001.4	7001.4	4768.4	7001.4
1.3	σ_x	7575.9	7575.9	7825.5	7575.8
	$\bar{\sigma}$	7556.9	7556.9	5162.8	7556.9
1.4	σ_x	7697.6	7697.6	8427.5	7697.7
	$\bar{\sigma}$	7601.2	7601.2	5559.8	7601.1
1.5	σ_x	7627.4	7627.4	9028.6	7627.5
	$\bar{\sigma}$	7673.1	7673.1	5958.2	7673.1

*1 Other entries of **d** and **h** are kept unity.

3.5 List of Symbols

NOMENCLATURE

Alphabetical Symbol	Description
A, B, C	Parameters in secant-Newton procedure
B	Strain-displacement matrix
C	Strain (or stress) projection operator
CH	Cayley-Hamilton matrix in polar decomposition
D	Material modulus matrix
D_{ijkl}	Fourth order tensor component of material modulus
dx	Differential volume (under integral sign)
F	Nodal force vector
F, G	Function indicators
h	Thickness for plates and shells
I	Functional indicator
I	Identity matrix (unit tensor)
J	Jacobian matrix for isoparametric transformation
K	Displacement stiffness matrix
M	Element basis function vector
M_K	Functional component of element basis function vector
N	Plasticity power law hardening parameter
N_i	Langrangian basis function associated with i-th node in an element
n	Number of dimensions
N_g	Total number of stress/strain sampling points in a given mesh
N_d	Number of displacement nodes
N_S	Number of stress nodes

Alphabetical Symbol	Description
P	Load at a given point
p, q	Singularity powers
r	Radial coordinate
$\underset{\sim}{R}, \underset{\sim}{R}^*$	Residual force vector
$\underset{\sim}{\mathrm{ROT}}$	Rotation tensor
$\underset{\sim}{S}$	Nodal stress vector
s	Line search parameter
$\underset{\sim}{U}$	Right stretch tensor
$\underset{\sim}{u}, \underset{\sim}{u}^*$	Displacement vector
$\underset{\sim}{u}_j$	Displacement vector component
V	Space for admissible displacement variation
$\underset{\sim}{v}_j$	Vector for BFGS update
W	Strain energy density
$\underset{\sim}{w}_j$	Vector for BFGS update
$\underset{\sim}{x}$	Position vector
x_j	Cartesian component of the position vector

Greek Symbols	Description
β	Conjugate gradient parameter
γ	Coefficient parameter in plasticity power law form
$\underset{\sim}{\gamma}_j$	Vector differences in residual load vectors for BFGS approach
δ_0, δ_1	Conjugate gradient parameters
$\underset{\sim}{\epsilon}$	Strain tensor
ϵ_{ij}	Strain tensor component

Greek Symbols	Description
θ	Tangential coordinate
λ	Load factor in arc-length method
ν	Poisson's ratio
π	Product indicator
ξ, η, ξ	Isoparametric Coordinates
$\underset{\sim}{\sigma}$	Stress tensor
σ_{ij}	Stress tensor component
Ω	Problem domain
$\partial\Omega$	Boundary of the domain

Sub- and Superscripts	Description
i, j, k, ...	Indices for vector and tensor component (when used as the subscripts); iteration and incrementation counter (when used as the superscripts)
I, J, K, ...	Nodal point counter
MAX	Maximum number
0	Initial quantities
S (Subscript)	Shear and transverse shear component
T (Subscript)	Tangent
R (Superscript)	Regular part indication
S (Superscript)	Singular part indication
T (Superscript)	Indicates transpose of matrix
-1 (Superscript)	Indicates inverse of matrix

Other	
$(\ )_{,j}$	Derivative with respect to x_j
$(\dot{\ })$	Derivative with respect to time

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